LA-UR-03-2088

Earth and Environmental Sciences Division (EES Division)

Science and Technology Assessment

and

Division Review Committee Meeting

May 12-14, 2003

Los Alamos, New Mexico

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Ideas That Change the World

CONTENTS

FOR FURTHER INFORMATION PLEASE CONTACT:

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PREFACE

The University of California (UC) operates the Los Alamos National Laboratory (LANL) for the Department of Energy (DOE). The contract provides for reviews, including various reports and annual reviews of about one-third of the portfolio by an external Division Review Committee (DRC).

The Earth and Environmental Sciences (EES) Division publishes biannual progress reports, most recently covering 2001 and 2002. The topics to be reviewed by the DRC on 12-14 May 2003 are shown in the agenda (-ii-), and the progress report provides much, but not all, of the written information required for that review. This document provides the additional information required for the annual DRC meeting.

Dates of previous EES/DRC meetings are: May 16-18, 1994; June 5-7, 1995; May 14-16, 1996; April 14-16, 1997; May 12-14, 1998; May 17-19, 1999; April 8-12, 2001; and April 2-4, 2002. (The DRC meeting for 2000 was cancelled due to the Cerro Grande fire.)

Agenda

EES DIVISION REVIEW COMMITTEE

Freeman Gilbert, Chair
Shlomo P. Neuman
Nafi Toksoz
Martinus (Rein) van Genuchten
Leland Younker
Rattan Lal
Veerabhadran Ramanathan
Alexandra Navrotsky
Jefferson Tester
Joanne Nigg
Tony Busalacchi
Leon Silver (Member Emeritus)

UC Technical Point-of-Contact
Jeffrey Dozier
Bernard Minster

May 12-14, 2003

Monday, May 12, 2003

7:30 - 8:00	Meet visitors in lobby of Best Western Hilltop House Hotel and escort to J. Robert Oppenheimer Study Center, Jemez/ Cochiti Rooms (TA-3, SM-207, Rms. 216/218)	Stella J. Ledbetter Deborah A. Pirkl
8:00 - 8:45	Welcome/Introductions • Review Agenda	Paul G. Weber
	SUMMARY TALKS (Performance Objective V)	
8:45 - 9:15	Atmospheric Sciences	James E. Bossert
9:15 - 9:45	Environmental	Donald D. Hickmott
9:45 - 10:15	National Security	Wendee M. Brunish
10:15 -10:35	BREAK	

Institutional Host:	Thomas J. Meyer, ADSR
Technical Host:	Paul G. Weber, EES-DO
Visit Planner:	Stella Ledbetter, CER-20/ Protocol
Food Service:	ARAMARK

10:35 - 11:05	Fossil Energy—Oil & Gas	Michael C. Fehler
11:05 - 11:35	Repository—WIPP	Ned Z. Elkins
11:35 - 12:05	Repository—Yucca Mountain	Paul R. Dixon
12:05 - 12:15	BREAK	
12:15 - 1:15	Working lunch *(by invitation only)* EES Post Docs and Students	Committee Members
1:15 - 1:30	BREAK	
1:30 - 5:00	***POSTER SESSION*** **(Performance Objective V)**	

Topical Areas:

Atmospheric Sciences

- Development of a New EMP Code at LANL — Jonah Colman
- Tropical Western Pacific 2001-2002 — William M. Porch, Larry A. Jones
- Exploring Wildfire Behavior with FIRETEC — Rodman R. Linn
- Confronting Models with Data: CFC Transport in the Ocean — Rainer Bleck

Environment—LANL

- Aqueous Environmental Geochemistry of Mortandad Canyon — Patrick Longmire
- Groundwater Pathway Analysis for the Pajarito Plateau — Kay H. Birdsell
- Tracing Environmental Processes at LANL Using Stable Isoptopes — Jeffrey M. Heikoop, Julianna Fessenden-Rahn
- Numerical Modeling of NAPL Source Zone Treatment Using LANL's ASCI Q Supercomputer — Peter C. Lichtner

Environment—NTS

- Colloid-Facilitated Transport in Fractured Rocks: Parameter Estimation and Comparison with Experimental Data — Andrew V. Wolfsberg, Phillip H. Stauffer
- Subsurface Geological Characterizations at Frenchman and Yucca Flats, Nevada Test Site: Implications to Hydrogeologic Investigations — Giday WoldeGabriel

Fossil Energy—Sequestration

- Carbon Analysis in Soils and Terrestrial Sequestration — David D. Breshears, Michael H. Ebinger
- CO_2 Injection in a Depleted Oil Reservoir in Hobbs, NM — Rajesh J. Pawar
- Stochastic Reservoir Simulations — Dongxiao Zhang
- Studies of the Consequences of Ocean Carbon Sequestration Using Los Alamos Models — Shaoping Chu

Institutional Host:	Thomas J. Meyer, ADSR
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	LDRD	
	• Neutron Scattering and the Non-Linear Acoustic Properties of Rocks	James A. TenCate
	• Technical Progress in the Development of Zero Emission Coal Technologies	Hans-Joachim Ziock
	• Preparing for a Hydrogen Economy: Sources, Sinks and Environmental Impacts	Thomas A. Rahn Manvendra K. Dubey
	Office of Science	
	• On Dynamic Nonlinear Elasticity and Small Strain	Paul A. Johnson
	• Wave Propagation in the Heterogeneous Earth	Michael C. Fehler
	• Vertical Transport and Mixing in the Stable Boundary Layer	Keeley R. Costigan
	Repository—WIPP	
	• An Apatite II Permeable Reactive Barrier to Remediate Pb, Zn, Cd, in Acid Mine Drainage At Success Mine	James L. Conca Marian Borkowski
	• The Actinide Chemistry and Repository Science Program in Support of the Waste Isolation Pilot Plant (WIPP)	Jean-Francois Lucchini
5:00 - 6:00	Committee Time (Closed Session: DRC only)	Committee Members
6:00 - 6:15	Escort visitors to Otowi Cafeteria	Stella Ledbetter
6:15 - 8:30	Working dinner *(by invitation only)* Dinner Speaker: Q Machine	 Andrew B. White
8:30 - 8:45	Escort visitors to Hilltop House Hotel	Stella J. Ledbetter

<u>Tuesday, May 13, 2003</u>

7:30 - 8:00	Meet visitors in lobby of Best Western Hilltop House Hotel and escort to J. Robert Oppenheimer Study Center, Jemez/ Cochiti Rooms (TA-3, SM-207, Rms. 216/218)	Stella J. Ledbetter Deborah A. Pirkl
	(Closed Session: DRC and named participants only)	
8:00 - 8:15	Introductions	Paul G. Weber
8:15 - 8:35	Welcome/Laboratory Overview	George P. Nanos, Jr.
8:35 - 8:50	Opening	William H. Press
8:50 - 9:00	Evaluation Process	James C. Porter, Jr.
9:00 - 9:30	SR and Laboratory Update	Thomas J. Meyer
9:30 - 9:45	Break	
9:45 - 10:45	Division-Overview and Update (Open Session) (Performance Objectives V, VII, VIII, and IX)	Paul G. Weber

Institutional Host:	Thomas J. Meyer, ADSR
Technical Hosts:	Paul G. Weber, EES-DO
Visit Planner:	Stella Ledbetter, CER-20/ Protocol
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10:45 - 11:00	IGPP, EES, LANL Relations	Gerald L. Geernaert
11:00 -11:15	New Initiatives	Paul G. Weber
11:15 - 11:45	Nuclear Weapons Effects Thrust (II.1, V)	Gregory A. Valentine
11:45 - 12:45	Working lunch (*by invitation only*) • Discussions with Science and Engineering Leadership Team (SELT)	 Committee SELT, et al.
12:45 - 1:15	Hard & Deeply Buried Targets Thrust (V)	Wendee M. Brunish
1:15 - 1:45	Water Resources Thrust (V)	Everett P. Springer
1:45 - 2:15	Carbon Management Thrust (V)	George D. Guthrie, Jr.
2:15 - 2:45	Homeland Security (IV)	Tom W. Meyer/ Wiley Davidson
2:45 – 3:00	Break	
3:00 – 4:00	Group Leader/Deputy Group Leader Discussions (Closed Session: DRC and named participants only)	Committee EES Group Managers
4:00 - 5:30	Committee Time (Closed Session)	Committee
5:30 - 6:30	LANL-Hosted Reception *(by invitation only)*	
6:30	Escort visitors to Best Western Hilltop House Hotel	Stella J. Ledbetter

<u>Wednesday, May 14, 2003</u>

7:15 - 7:30	Meet visitors in lobby of Hilltop House Hotel and escort to J. Robert Oppenheimer Study Center, Jemez/ Cochiti Rooms (TA-3, SM-207, Rms. 216/218)	Stella J. Ledbetter Deborah A. Pirkl
7:30 - 9:30	Executive Session (Closed Session: named participants only) (DRC report to Laboratory Management)	Committee Members George P. Nanos, Jr. William H. Press Thomas J. Meyer Allen Hartford, Jr. James C. Porter Paul G. Weber
9:30 - 10:45	EES Division Management Out-brief	
10:45 - 11:30	Close Out (Open Session)	EES Division
11:30	Meeting Adjourned Escort visitors to Best Western Hilltop House Hotel	 Stella J. Ledbetter

Institutional Host:	Thomas J. Meyer, ADSR
Technical Hosts:	Paul G. Weber, EES-DO
Visit Planner:	Stella Ledbetter, CER-20/ Protocol
Food Service:	ARAMARK

1.0 ORGANIZATIONAL PROFILE

Division Leader: Paul G. Weber

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Deputy Division Leader: Vacant

Organization and reorganization

The Earth and Environmental Sciences (EES) Division was established in 1989. In late 2000 the Division underwent a review by the Associate Director for Strategic and Supporting Research (ADSSR), which resulted in a **structural** reorganization of the group structure and establishment of the Science and Engineering Leadership Team (SELT). The Division Director left at that time, and nine months passed before a new Division Leader was appointed. Following some familiarization time, we started a process of **cultural** changes to build on the structural changes. This process was driven by a representative team of division members who identified issues deemed to be worthy of the attentions of the whole Division. Through communications, meetings of the Division, and a detailed questionnaire, we were able to reach consensus on areas for potential improvement. These included the need for defining a new vision and mission; a new analysis of our capabilities; a need to better engage in program development; and improvements in our communications, including Web pages, publications, and seminars. The next several segments reflect actions and changes based on the strong consensus reached by the majority of Division members who engaged in the process.

Vision

To provide outstanding scientific and engineering leadership, basic and applied research and development, and applications that benefit our Environment, Energy, and National Security.

Mission

Using our capabilities in earth and environmental sciences and engineering, we provide solutions to complex problems of importance in the Environment, Energy, and National Security.

Capabilities

This list of capabilities was developed through a questionnaire in which Division members who engage in technical work were able to define the mix of capabilities to which they contribute. For example, a mathematician engaged in hydrology could identify a mix of 43% mathematics and 57 % hydrology. Adding all these allocations leads to the highest ranked capabilities (in alphabetical order):

Atmospheric & Oceanic Sciences
Computational Science / Mathematics
Ecology
Geochemistry / Geomaterials
Geology
Geophysics / Seismology
Hydrology
National Security Science / Technology
Technical Leadership / Management

Program Elements

The main program elements and research highlights for the Division are described in detail in the Progress Report. Our largest programs are: Yucca Mountain, Waste Isolation Pilot Plant Carlsbad Operations, Tropical Western Pacific Sites of the DOE Atmospheric Radiation Measurements Program, Ground-based Nuclear Explosion Detection for DOE/NA-22, Nuclear Weapons Effects, Environmental Restoration for DOE/EM, and portfolios of smaller projects for the DOE Office of Fossil Energy and Office of Science, Laboratory Directed Research and Development, and others. With the transition to program/line integration in the Division, we will have many more opportunities to interface directly with the sponsors to ensure that they continue to be pleased with our efforts, and to provide us with a clearer insight to their unmet needs.

Groups and Integrated Program Functions

As a part of the December 2000 reorganization, the Division moved to a structure of six groups with each group covering a particular set of capabilities. The Institute for Geophysics and Planetary Physics continued to report to the EES Division Director. This structure was in place until October 1, 2002, when we merged our smallest Los Alamos-based group, EES-10, into two other groups (EES-8 and EES-9), mostly for cost efficiency reasons. Detailed descriptions of each of the Groups, their capabilities, and examples of recent research are found in the Progress Report.

It was also clear that a weakness in EES was the fact that the Division relied on Program Offices in other parts of the Laboratory to interface with the sponsors. The model in some other parts of the Laboratory was to align the Program and Line functions within the Divisions: this has worked very well, for example, in the Nonproliferation and International Security Division since its formation in 1993. We initiated discussions on this topic, and after lengthy deliberations, gained agreement on moving Program functions into EES Division. Specifically, the Yucca Mountain and Waste Isolation Pilot Plant Program Offices moved with the dissolution of E-Division in April 2002. Effective

1 October 2002, we took over the program management of most of the Carbon Sequestration and Fossil Energy portfolios. Additionally, we have expanded the scope of our efforts as program managers for the environmental elements of the DOE Office of Science Programs to incorporate working directly on the new US Climate Change Initiative. With these changes, we now have direct program responsibility for over half of the work in the Division, and we believe that we are better positioned for growth.

Beyond maintaining and growing our existing programs, we see major opportunities in several areas. The choice of these areas is based on evaluations by the Division staff, in concert with Program Managers and other leaders. We make investments of program development funds in these so-called "Thrusts", and develop them in collaboration with others. A brief description of each Thrust follows.

Carbon Management

This thrust is broad in terms of both technical capabilities and sources of funding. LANL performs research, development, science, and diagnostics in virtually all approaches of carbon management and sequestration strategies under investigation. These include geological, clathrates, terrestrial, CO_2 mineralization, ZECA (Zero Emissions Coal Alliance), air extraction of CO_2, seismic imaging, and ocean biogeochemistry. It is noteworthy that LANL is making strong technical contributions in all key areas of carbon management and sequestration, and some long-term approaches and monitoring technologies were conceived at LANL. The intent of the carbon thrust is to capitalize on LANL's breadth, depth, niche, and vision and its balance of short and long-term carbon management approaches to generate a strong, large, and vibrant program. This effort is partially supported by Institutional Program Development funds, and is performed in strong collaboration with the new Office of Energy and Environment Initiatives.

Water

The thrust encompasses program development in the following areas: water for energy, DOE water cycle initiative, water security, NICHES, NASA interactions, and water technology. EES has been actively pursuing these initiatives for at least two years. Currently, EES PIs are involved in an LDRD/DR on the water cycle, which highlights our capabilities in coupled modeling with high-performance computing. EES was also successful in obtaining DOE funding to support the Water Cycle Pilot Project. Over the past year, workshops were held with stakeholders from industry and state government to identify critical issues in the allocation and use of water in energy production. Outcomes of these workshops were incorporated in a Senate bill, which was funded for desalination and arsenic removal (at Sandia) but not for predictive modeling (at LANL). Nevertheless, EES has been encouraged to continue the process of program development. This effort is partially supported by Institutional funds, and is performed in strong collaboration with the new Office of Energy and Environment Initiatives.

Nuclear Weapon Effects (N.W.E.)

The primary aspects of this thrust are:

(a) Weapons functions,
(b) Propagation path effects (earth, atmospheric),
(c) Sensors, and
(d) Target.

There has been a steady decline in these capabilities at all of the weapons labs (LANL, LLNL, SNL) since the end of the cold war. The interest from NNSA, DTRA, and management has recently increased. NNSA and DTRA are the primary customers. Divisions involved in this Thrust are EES, ESA, D, NIS, T, and X, and the other institutions involved are SNL and LLNL. Applications that require NWE support include

(a) Survivability of US weapons in hostile environments,
(b) Lethality of US weapons,
(c) Detectability of foreign tests,
(d) Containment,
(e) Vulnerability of the homeland.

Three workshops have been held focusing on sub-areas of NWE:

(a) Solid Earth effects,
(b) Space and high altitude effects,
(c) Low altitude effects.

The workshops included individuals from each Laboratory. As a result of these efforts, the cognizant Associate Directors at all three Labs endorsed a planning effort that includes a roadmap and total funds required. The plan is due in February 2003 for consideration in the 2005-09 budget planning.

Hard & Deeply Buried Targets

The defeat of hard and deeply buried targets has been a thrust within EES for about 18 months. Many targets worldwide require careful definition both in terms of the geology and the infrastructure that is hidden or protected by the geology. Geologic models definition and modeling weapons effects are the primary motivation behind EES involvement in this effort. Additional high fidelity modeling of facilities is needed to assess target vulnerability. The geologic models must include topography, lithology, target geometry, constitutive models for each rock type, and associated uncertainties for each of the model fields. Once geologic/infrastructure models are defined, hydrodynamic and seismic forward modeling of defeat weapons are applied to the model to determine the effects on the hardened target.

To date, the thrust at LANL has defined a unique approach that involves members from D, EES, ESA, and X Divisions at LANL and DTRA. This approach includes a model definition using tools that are accessible to the LANL primary customers, STRATCOM and DIA, with meshing and forward modeling by EES and D division on the geologic structures and facilities. The thrust members have attended many technical meetings and produced publications.

Homeland Security

As of the end of 2002, the Center for Homeland Security is being established at LANL, as the main interface to, and reflecting the structure of, the new Federal Department of Homeland Security, which will officially commence operations in late February 2003. As such, the situation is fluid. However, in preparation for moving quickly when opportunities arise, we have designated EES Division points of contact to each of the Associate Directors in CHS, namely: Chemical / Biological, Nuclear and Radiological Security, and Infrastructure.

Summary of Thrusts

We will continue to review our Thrusts to ensure that we are investing precious program development dollars wisely.

Science and Engineering Leadership Team (SELT):

The SELT was established as a part of the EES re-organization. The Vision for SELT is: "To help EES technical staff become more effective at obtaining research and development funds."

The SELT consists of between six and ten members, including no more than one Group Leader or Deputy Group Leader. In May of each year the Division Leader, with input from SELT and the Group Leaders, appoints new members. They serve staggered two-year terms. Vacancies during the year may be filled at the discretion of the Division Leader.

Specifically, the SELT does the following:
Gather and share information from LANL program managers,
Promote collaborations,
Improve skills in program development and leadership,
Provide information to EES staff on avenues for building projects and programs and promoting new ideas,
Aid EES staff in developing high-quality proposals, and
Assist in placing EES staff on LANL technical committees.

SELT meets weekly and meeting summaries are available on-line.

Current SELT members

Claudia Lewis, EES-9 (Chair)
James Bossert, EES-2
Dave Breshears, EES-2
Rodman Linn, EES-2
Cathy Wilson, EES-2
Manvendra Dubey, EES-6
Steen Rasmussen, EES-6
Paul Rich, EES-9
Paul Johnson, EES-11
Robert Swift, EES-11
Chris Bradley, EES-11 (alternate)

Administrative Assistance: Rhonda Holloway, EES-DO

Past SELT members:
Mike Fehler, EES-11
George Guthrie, EES-6
Frank Perry, EES-9
Gilles Bussod, no longer at LANL
Aaron Velasco, no longer at LANL

Insitute of Geophysics and Planetary Physics

EES includes the Institute of Geophysics and Planetary Physics (IGPP), which supports basic research in astrophysics; geophysics; and oceanic, atmospheric, and magnetospheric sciences.

Yucca Mountain Project Team Distinguished Performance Award

Director John Browne announced in October 2002 that the Yucca Mountain Project Team would receive a Large Team Distinguished Performance Award. This is a very high and well-deserved honor! Quoting from the nomination memo:

"The fact that the Secretary of Energy was able to recommend Yucca Mountain in the face of daunting political challenges is a testament to the outstanding science that the Yucca Mountain Program has been able to deliver. The Yucca Mountain Program Staff has assisted in completing a major political and technological milestone by resolving a problem that has impact at the national level, bringing distinction to Los Alamos National Laboratory."

"The nominees of this award have truly excelled in their performance of the broad spectrum of scientific, engineering, technical, administrative, and management activities needed to provide the science, credibility, and defensible documentation that will allow DOE to move forward to the License Application for our nation's first high-level nuclear waste repository, Yucca Mountain."

Geographic Information Systems Team Award

The Geographic Information Systems Lab (GISLab) was selected to receive a Special Achievement in GIS" award at ESRI's 22nd Annual User Conference, in recognition of GIS efforts in support of the Cerro Grande Rehabilitation Project. This award is given to select user sites around the world in recognition of their outstanding work in the GIS field. GISLab was chosen to receive this prize from over 100,000 user sites worldwide. In May 2000, the Cerro Grande Fire swept through Los Alamos, NM, burning more than 48,000 acres, and causing evacuation of the national Laboratory and town. GIS was an integral part of response during the fire, and continues to be used for restoration and environmental monitoring under the Cerro Grande Rehabilitation Project. This prize was awarded to the GISLab and the many colleagues at Los Alamos National Laboratory who contributed to these GIS efforts.

Personnel

The accomplishments of EES Division result from the talent and dedication of its people. Table 1 shows EES Division employees as of March 1, 2003, and preceding years. If contractors are included, the total EES Division workforce is approximately 317. The technical staff members, technicians, postdoctoral fellows and graduate students are the technical workforce of the division, and the sum of these employees has remained relatively constant at slightly under 300 for the past five years. Post-doctoral fellows and graduate research assistants participate as full colleagues on many projects, both basic and applied; their involvement is vital to our scientific health. The number of post-doctoral fellows/research associates has greatly improved this year. Nine new technical staff members (scientists), one new post-doctoral fellow, and five post-doctoral research associates joined EES during Calendar Year (CY) 2002 *(see Appendix B.9 for profiles of these individuals)*.

Table 1. Employee Profile

(Personnel numbers are as of March 1 of the year indicated.)

	1999	2000	2001	2002	2003
Technical Staff Members	148	145	139	144	155
Post-Doctoral Fellows/ Research Associates	11	10	14	13	17
Technicians	30	30	28	33	26
Graduate Students	23	19	16	30	26
OS/GS	21	21	22	20	15
SSM	11	10	8	12	13
Undergraduate and High School Student	38	37	26	25	35
Total	282	272	253	277	287

Programs, Funding and Customers

Fiscal Year (FY) 2003 funding for EES Division is $64 million as of March 2003. The total funding for FY 2002 was $64.8 million. EES program and project areas, key customers and funding levels are shown on Table 2.

Table 2. Major EES Programs, FY 2001-2002

Programs/Projects	FY02 Funding (M$)	FY03 Funding (M$)	Customer
Los Alamos Environmental Restoration	6.7	4.7	DOE Office of Environmental Management
Waste Isolation Pilot Plant	4.3	8.3	DOE Office of Environmental Management
Yucca Mountain Project	9.1	10.0	DOE Office of Civilian Radioactive Waste Management
Arms Control Research	7.6	7.9	DOE Office of Nonproliferation and National Security
Fossil Energy Projects	5.7	5.4	DOE Office of Fossil Energy
Global Climate Research	8.6	9.0	DOE Office of Biological & Environmental Research (OBER)
Basic Energy Sciences	2.3	2.3	DOE Office of Basic Energy Research (OBES)-Geosciences
Weapons Research and Development	5.4	4.8	DOE Defense Programs, CIT--technology transfers
Laboratory Directed Research and Development	3.3	4.5	Los Alamos Science and Technology Base Program
IGPP, Volcanology	2.2	1.0	Los Alamos Science and Technology Base Program
Other DOE Facilities	3.4	3.5	DOE
Other Research Projects	2.1	1.2	Other Federal Agencies: DOD, NASA, and others
Other Funding Source	1.9	0.9	Recharges, ESS, IBD, etc.
CG Fire Related Work	2.2	0.5	DOE
Total	**64.8**	**64.0**	

Facilities and Equipment

In addition to people, access to modern laboratory, field and computing equipment is critical to our capabilities. EES uses and is responsible for approximately 2,200 items of equipment with a total purchase cost of approximately $20,000,000. The laboratory equipment includes geochemical instruments for rock, mineral and water analyses; geophysical laboratories for electrical and acoustical properties measurements; a drilling research laboratory; electrical/mechanical shops for the fabrication of borehole instruments; a geographic information system; and a greenhouse, wet chemistry lab and related facilities for ecological studies. The field equipment includes portable seismometers and other exploration geophysical equipment, a permanent seismic network in the Los Alamos areas, drilling rigs (including mechanical shops), lidar and meteorological measurement equipment, and caisson clusters. Our computing equipment includes personal computers, networked scientific workstations, and—through other organizations—access to institutional computing resources. EES occupies approximately 83,000 square feet of office and laboratory space at Los Alamos.

In Nevada, EES is responsible for key activities associated with the construction and operation of underground experimental facilities associated with the Yucca Mountain Project, and some of the equipment and instruments associated with this work.

In Carlsbad, New Mexico, EES is responsible for key activities associated with the operation of the Waste Isolation Pilot Plant (WIPP), and state-of-the art equipment, such as laser photoacoustic spectrometry and LANL's mobile Contaminant Analysis Automation (CAA) laboratory.

Organizational Structure

The organization of the Laboratory is shown in Figures 1, and 2. EES is one of 16 technical divisions at the Laboratory. EES consists of six groups and the Institute of Geophysics and Planetary Physics (IGPP). EES is the Laboratory institutional home for the IGPP.

The organizational structure of EES is shown in Figure 3. EES operations are highly decentralized, with individual group leaders responsible for management of research, and for operational matters such as fiscal accountability, safety and security of operations, and regulatory compliance.

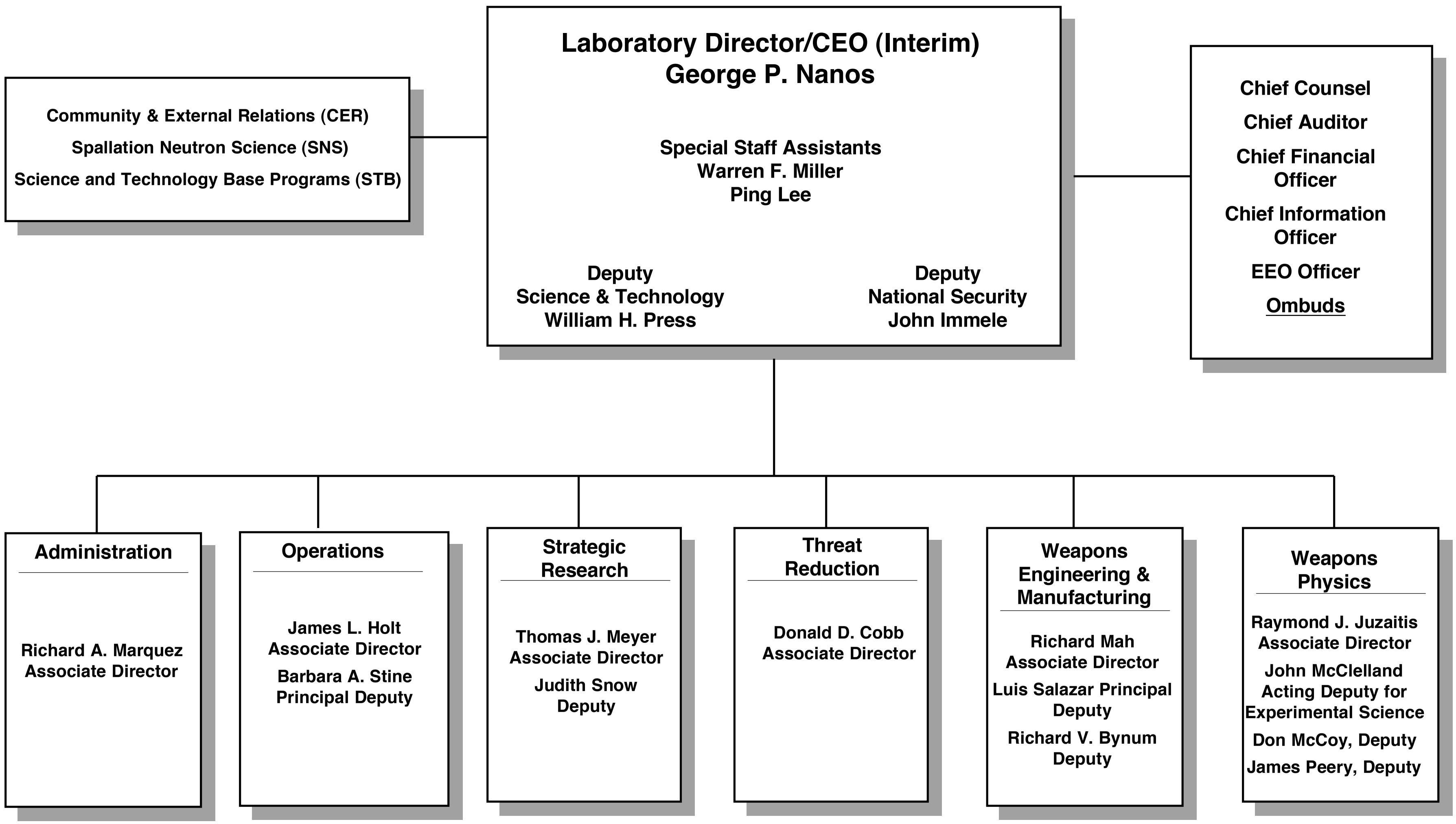

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Figure 1

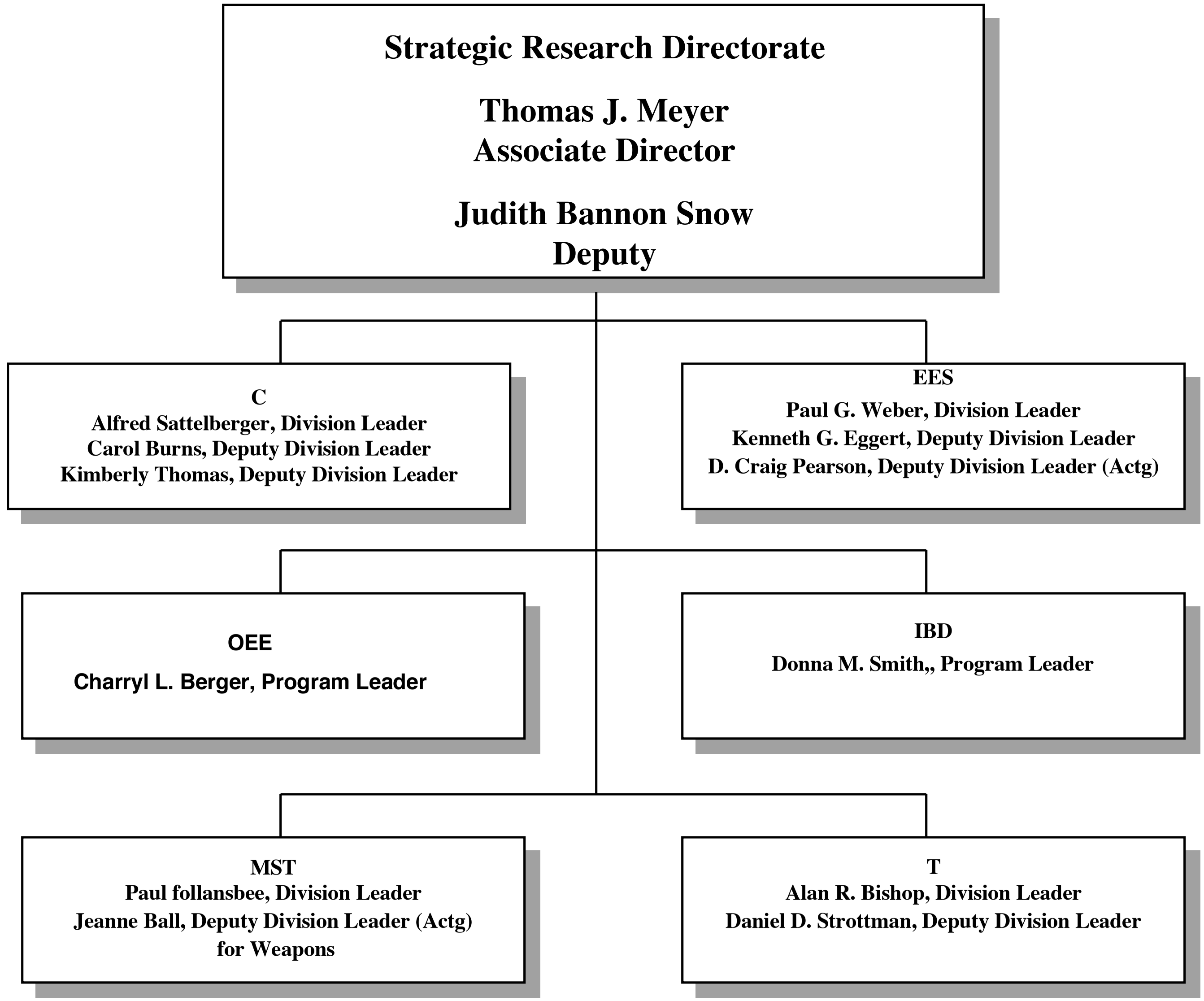

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Figure 2

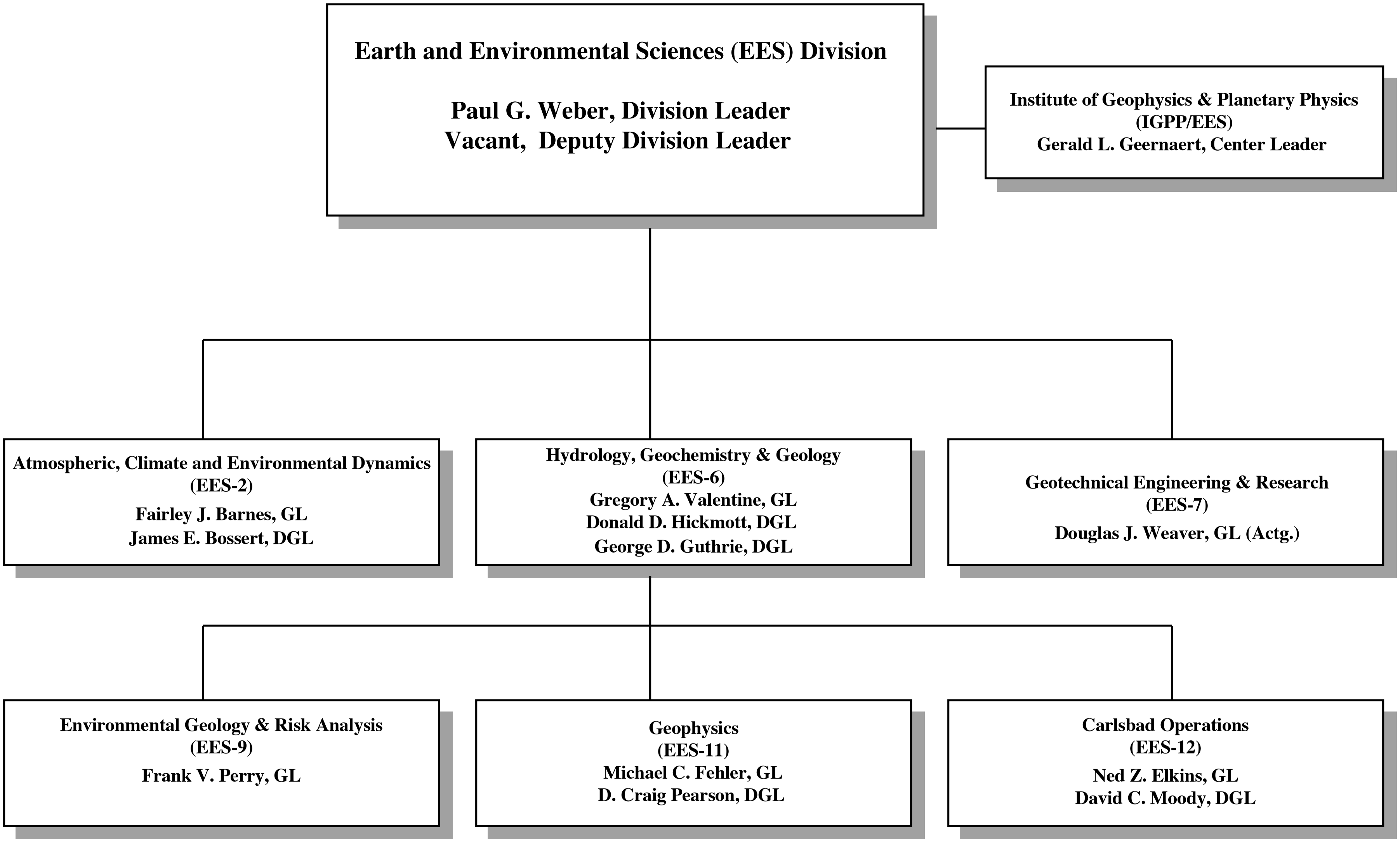

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Figure 3

University	Staff Member	Group	Type of Contact	Discipline for Recruiting/ Collaborating
Amherst College	Don Hickmott	EES-6	Advisor, Thesis Committee, Colleagues	Earth Sciences
Bakersfield	Claudia Lewis	EES-9	Faculty; Funding requests pending for Collaborations	Geology, Tectonics, Paleoseismology
Brown University	Claudia Lewis	EES-9	Alumni activities	Geology
Cal State	Claudia Lewis	EES-9	Faculty; Funding requests pending for Collaborations	Geology, Tectonics, Paleoseismology
California Institute of Technology	Paul Weber	EES-DO	Consultant--Division Review Committee Member, Leon Silver	Geology, Geochemistry
California Institute of Technology	Claudia Lewis	EES-9	Contact with Faculty and Students	Geology, Tectonics, Paleoseismology
California Institute of Technology	Manvendra Dubey	EES-6	Alumni, Student, Postdoc, Research Collaborations	Environmental Science, Chemistry, Physics
Colorado School of Mines	Peng-Hsiang Tseng	EES-6	Collaborations	Hydrology, Water Resources, Environmental Sciences
Colorado School of Mines	Howard Hanson	EES-8	HR-5 Recruiting and Career Fairs	Environmental Sciences
Colorado State University	Howard Hanson	EES-8	HR-5 Recruiting and Career Fairs	Environmental Sciences
Columbia	Manvendra Dubey	EES-6	Alumni, Student, Postdoc, Research Collaborations	Environmental Science, Chemistry, Physics
Desert Research Institute	Claudia Lewis	EES-9	Collaborations	Geology, Tectonics, Paleoseismology
Eastern Illinois University	Carl Gable	EES-6	Technical Collaboration with Faculty	Earth Science, Geology

University	Staff Member	Group	Type of Contact	Discipline for Recruiting/ Collaborating
Golden West College	Scott Baldridge	EES-11	Contacts with Faculty	Geophysics
Harvard University	Claudia Lewis	EES-9	Faculty	Geology
Harvard University	Carl Gable	EES-6	Alumnus, Technical Collaboration with Faculty	Earth Science, Applied Physics, Geophysics
Harvard University	Manvendra Dubey	EES-6	Alumni, Student, Postdoc, Research Collaborations	Environmental Science, Chemistry, Physics
Indiana University	Carl Gable	EES-6	Technical Collaboration with Faculty	Earth Science, Geology
Louisiana State University	Carl Gable	EES-6	Technical Collaboration with Faculty	Earth Science, Geology
MIT	Paul Weber	EES-DO	Nafi Toksoz, Consultant--Division Review Committee Member	Geophysics
MIT	Michael Feher	EES-11	good ties, Chair of Editorial Board	Geophysics, Geology
NM Highland	Manvendra Dubey	EES-6	Alumni, Student, Postdoc, Research Collaborations	Environmental Science, Chemistry, Physics
NM State Univ.	Michael Feher	EES-11	good ties, Chair of Editorial Board	Geophysics, Geology
NM State Univ.	Scott Baldridge	EES-11	Contacts with Faculty	Geophysics
NM Tech	Claudia Lewis	EES-9	Collaborations	Geology, Tectonics, Paleoseismology
NM Tech	Michael Feher	EES-11	Adjunct Faculty	Geophysics, Geology
NM Tech	Manvendra Dubey	EES-6	Alumni, Student, Postdoc, Research Collaborations	Environmental Science, Chemistry, Physics
NM Tech,	Michael Feher	EES-11	good ties, Chair of Editorial Board	Geophysics, Geology
Ohio State University	Paul Weber	EES-DO	Rattan Lal, Consultant--Division Review Committee Member	Soil Physics

University	Staff Member	Group	Type of Contact	Discipline for Recruiting/ Collaborating
Penn. State University	Douglas ReVelle	EES-8	Research Collaborator (J. Mathews)	Ionospheric Physics, Atmospheric Sciences
Purdue	Scott Baldridge	EES-11	Contacts with Faculty	Geophysics
Purdue University	Carl Gable	EES-6	Technical Collaboration with Faculty	Earth Science, Geophysics
Reed College	Michael Feher	EES-11	Undergrad Thesis Advisor	Geophysics, Geology
San Diego State University	Scott Baldridge	EES-11	Contacts through SAGE	Geophysics
Southern Methodist University	D. Craig Pearson	EES-DO/ EES-11	Alumnus, continuing contact with Geology Department	Geology, Geophysics, Seismology
Stanford,	Manvendra Dubey	EES-6	Alumni, Student, Postdoc, Research Collaborations	Environmental Science, Chemistry, Physics
Stockholm University, Stockholm, Sweden	Douglas ReVelle	EES-8	Research collaborator (E.D. Nillson)	Atmospheric Sciences
UC Berkeley	Carl Gable	EES-6	Alumnus	Earth Science, Geophysics
UC Davis	Claudia Lewis	EES-9	Faculty; Funding requests pending for Collaborations	Geology, Tectonics, Paleoseismology
UC Davis	Paul Weber	EES-DO	Alex Navrotsky, Consultant--Division Review Committee Member	Physics and Chemistry of Minerals, Geochemistry, solid State chemistry, Materials Science
UC Irvine	Howard Hanson	EES-8	IGPP proposal joint with Faculty Member	Environmental Sciences
UC Los Angeles	Carl Gable	EES-6	Technical Collaboration with Faculty	Earth Science, Geophysics
UC Riverside	Scott Baldridge	EES-11	Contacts with Faculty	Geophysics
UC Riverside	Peng-Hsiang Tseng	EES-6	Collaborations	Hydrology, Water Resources, Environmental Sciences

University	Staff Member	Group	Type of Contact	Discipline for Recruiting/ Collaborating
UC San Diego, Scripps Institute of Oceanography	Paul Weber	EES-DO	V. Ramanathan Consultant--Division Review Committee Member	Geophysical Sciences, Applied Ocean Sciences, Climate and Atmospheric Sciences
UC San Diego--IGPP	Paul Weber	EES-DO	Freeman Gilbert, Consultant--Division Review Committee Member	Geology, Geophysics
UC Santa Barbara	Douglas ReVelle	EES-8	(Alumnus, Adjunct, etc.): Research Collaborator-IGPP grant (T. Tanimoto)	Earth Sciences, Seismology, Atmospheric Sciences
UC Santa Cruz	Michael Feher	EES-11	good ties, Chair of Editorial Board	Geophysics, Geology
UC Santa Cruz	Scott Baldridge	EES-11	Collaboration	Geophysics
UC Santa Cruz.	Philip Stauffer	EES-6	Associate Professor	Hydrogeology
UCLA	Douglas ReVelle	EES-8	Research Collaborators (J. Wasson, J.-P. Williams)	Earth Sciences, Seismology, Planetary Atmospheres
Univ. Alabama	James Stalker	EES-8	Alumnus	Atmospheric Sciences & Mechanical Engineering
Univ. Arizona	Velimir Vesselinov	EES-6	Thesis advisor	Hydrology and water resources.
Univ. Arizona	James Stalker	EES-8	Mentor (through MentorNet) Undergrad. Student	Earth & Planetary Sciences
Univ. Arizona	Paul Weber	EES-DO	Shlomo P. Neuman, Consultant--Division Review Committee Member	Civil/Geotechnical Engineering, Hydrology, Water Resurces
Univ. Arizona	Steve Taylor	EES-11	Adjunct (Prof. Terry Wallace)	NNSA/ROA funded contract

University	Staff Member	Group	Type of Contact	Discipline for Recruiting/ Collaborating
Univ. Colorado Boulder	Howard Hanson	EES-8	HR-5 Recruiting and Career Fairs	Environmental Sciences
Univ. Hawaii, Manoa	Peng-Hsiang Tseng	EES-6	Collaborations	Hydrology, Water Resources, Environmental Sciences
Univ. Michigan (Ann Arbor)	Douglas ReVelle	EES-8	Colleague (S. Atreya)	Atmospheric Physics, Ionospheric Physics, Planetary Atmospheres, Magnetospheric Physics
Univ. New Mexico	Fraser Goff	EES-6	Adjunct Faculty	Earth Sciences
Univ. New Mexico	Don Hickmott	EES-6	Advisor, Thesis Committee, Colleagues	Earth Sciences
Univ. New Mexico	Claudia Lewis	EES-9	Adjunct Associate Professor	Geology
Univ. New Mexico	Scott Baldridge	EES-11	Contacts with Faculty	Geophysics
Univ. New Mexico	James Stalker	EES-8	Adjunct Faculty in the Earth and Planetary Sciences Department (UGS, GS)	Mechanical Engineering
Univ. New Mexico	Fraser E. Goff	EES-6	Adjunct Faculty, Dept. Earth Sci.	Earth Sciences
Univ. New Mexico	Gregory Valentine	EES-6	Adjunct Faculty, Dept. Earth Sci.	Earth Sciences
Univ. New Mexico	Kenneth H. Wohletz	EES-11	Adjunct Faculty, Dept. Earth Sci.	Earth Sciences
Univ. New Mexico	Scott Baldridge	EES-11	Teaching Class at Main Campus (Tobias Fisher), Dept.Earth & Planetary Sciences	Petrology
Univ. of Illinois Urbana-Champaign	Hari Viswanathan	EES-6	Professor	Hydrology, Env. Engr.

University	Staff Member	Group	Type of Contact	Discipline for Recruiting/ Collaborating
Univ. of Miami.	Howard Hanson	EES-8	Alumni	Environmental Sciences
Univ. of Missouri	Jeane Fair	EES-10	Alumnus	Ecology
Univ. of Texas	Scott Baldridge	EES-11	Contacts with Faculty	Geophysics
Univ. of Wisconsin	Scott Baldridge	EES-11	Contacts with Faculty	Geophysics
Universite Pierre et Marie Cuire, Paris, France	Jeane Fair	EES-10	Collaboration	Ecology
University of Leeds, Yorkshire, England	Carl Gable	EES-6	Technical Collaboration with Faculty	Earth Science, Geophysics
University of Paris 6&7	Paul A. Johnson	EES-11	(Alumnus, Adjunct, etc.) Visiting Professor	Geophysics General, Acoustics, Nonlinear Dynamics
University of Puerto Rico--Mayaguez	James Stalker	EES-8	Adjunct Faculty, Dept. of Mechanical Engineering (UGS, GS)	Mechanical Engineering
University of Western Ontario, London, Ontario, Canada	Douglas ReVelle	EES-8	Research Collaborator (P. Brown)	Atmospheric Physics and Dynamics, Earth Sciences
USDA-ARS, Salinity Laboratory	Paul Weber	EES-DO	M.T. van Genuchten Consultant--Division Review Committee Member	Soil Physics
Virginia Polytechnic Institute & State Univ. (Virginia Tech).	James Aldrich	EES-6	Advisory Board	Geological Sciences

Appendix A: Abstracts

#1 DEVELOPMENT OF A NEW EMP CODE AT LANL

Principal Investigator: Robert Roussel-Dupre, EES-2

Co-Investigators: Jonah Colman, EES-2
Laurie Triplett, EES-2
Bryan Travis, EES-2

A new code for modeling the generation of an electromagnetic pulse (EMP) by a nuclear explosion in the atmosphere is being developed. The source of the EMP is the Compton current produced by the prompt radiation (g-rays, X-rays, and neutrons) of the detonation. As a first step in building a multidimensional EMP code we have written a kinetic code, Plume, to model the transport of energetic electrons in air.

The Plume code solves the relativistic Fokker-Planck equation over a specified energy range that can include ~3 keV to 50 MeV and computes the resulting electron distribution function at each cell in a 2-D spatial grid. The Plume code employs a spherical coordinate system in momentum space and a cylindrical coordinate system in configuration space. The ‘z’ axes of the momentum and configuration spaces are assumed to be parallel; we are currently assuming complete spatial symmetry around the ‘z’ axis.

Primary (or energetic) electrons are allowed to transport, scatter, and experience Coulombic drag. Secondary electrons are also produced through primary ionization. Positive and negative ions are tracked, and the processes of two and three body dissociative attachment, radiative and dissociative recombination, detachment by O_2, N_2, and O_2 ($a^1\Delta_g$), and ion-ion recombination are included.

Microwave attenuation and optical emissions can also be calculated with the output of the Plume code. Here we report on recent results simulating an electron beam propagating at three different atmospheric pressures. Some experimental data are also discussed, and the relevance of quenching by water vapor is considered.

External Reviews: None

Collaborators: None
Publications: None

#2 TROPICAL WESTERN PACIFIC 2001–2002

Principal Investigators: Bill Porch, EES-2
Larry Jones, EES-2

During the 2001–2002 period, the important scientific progress centered around the beginning of the 2002 El Niño and its effect on the Atmospheric Radiation Measurement (ARM) Program's research sites in the Tropical Western Pacific (TWP) region. The combination of this event, supplemental remote sensing data from the DOE Multispectral Thermal Imaging Satellite (MTI), and the more recent Atmospheric Infra-Red Sounder (AIRS) component of the AQUA satellite are providing insights into the climatically important but poorly understood TWP region.

The 2002 El Niño affected predominant wind directions on Nauru Island. In 2000 the winds blew mostly from the east. In contrast, during the 2002 El Niño the wind directions were almost evenly distributed between east and west. In 2000, the MTI images of cloud trails from Nauru Island were combined with numerical cloud modeling, improving our understanding of the sensitivity of boundary layer clouds in tropical regions to perturbation. This model study showed that mechanical turbulence generated by the interception of the predominant wind by this small island (3 km diameter and 65 m high) can be enough under some circumstances to generate a cloud trail. However, comparison between nighttime and daytime images of the Nauru cloud trail indicates that in most cases convective turbulence by daytime island heating is more effective in forming the island cloud.

The ARM Program also established its third TWP Atmospheric Radiation and Cloud Station (ARCS) in Darwin, Australia, whose operations began in April 2002. The ARM Program chose Darwin because its climate regimes (i.e., dry continental, transitional period, and monsoonal regimes) are of specific interest for studies on atmospheric radiation and clouds. Darwin is also associated with existing scientific programs of the Australian Bureau of Meteorology (BOM) and the Commonwealth Scientific and Industrial Research Organization (CSIRO)—a rich research collaboration beneficial to all programs involved.

External Reviews: None

Collaborators: DOE Atmospheric Radiation Measurement Program participants

Publications: None

#3 EXPLORING WILDFIRE BEHAVIOR WITH FIRETEC

Principal Investigators: Rodman Linn, EES-2
Jon Reisner, EES-2
Judith Winterkamp, EES-2

Co-Investigators: Michael Steinzig, EES-2
Carleton Edminster, USDA Forest Service, Rocky Mountain Research Station
Michael Bradley, LLNL

LANL has been developing a physics-based wildfire model, FIRETEC, for the purpose of assisting decision makers concerned with wildfires and controlled burns. FIRETEC models the driving processes in a wildfire by solving a coupled set of partial differential equations that describe the conservation of mass, momentum, energy, species, and turbulence. The philosophy behind the development of FIRETEC is that a physics-based model of this type will be applicable to a variety of complex wildfire situations that empirically based wildfire models cannot represent. In addition, it is envisioned that in the future FIRETEC will be able to explain thresholds in wildfire behavior, helping determine ideal fuel-thinning strategies.

The ability to study fundamental wildfire behavior and model complex wildfire situations meets a national need for better understanding of wildfire behavior and its response to different environmental conditions. In addition to building a wildfire modeling capability, the work leading to the development of FIRETEC has increased EES capabilities in dispersion modeling and fine-scale atmospheric modeling.

In recent months, FIRETEC's developments have been focused in several areas. The first area of focus is the incorporation of the U.S. Forest Service data pertaining to discrete trees. This data is being used to create stands of trees for fire simulations. This is an important step because it will allow us to examine specific thinning strategies and the thresholds that dictate a fire's ability to become a crown fire.

Another focus area has been generating a framework that will allow for the testing of generalized rules regarding grass density variations. This is an important framework to have because the ability to model realistic stands of trees and fires that exist on the floor of a canopy depends upon the ground fuels and their distribution with respect to the trees.

In collaboration with the University of California Berkeley, we have begun using FIRETEC to examine trajectories of lofted firebrand. FIRETEC's 3-D representation of fire-influenced winds is an ideal tool for studying this phenomenon.

We are also using FIRETEC to study the influence of wind gusts on fire behavior. Initial tests show that in some situations strong fluctuations in the wind field have very significant effects on the average spread rate even in situations where the average wind velocity is unchanged from the constant wind situation.

External Reviews:	None
Collaborators:	Patrick Pagni, University of California Berkeley Mark Finney, USDA Forest Service, Rocky Mountain Research Station David Weise, USDA Forest Service, Pacific Southwest Research Station
Publications:	Linn, R.R., et al., "Studying Wildfire Using FIRETEC," *Int. J. Wildland Fire* **11**, 1–14 (2002).

#4 CONFRONTING MODELS WITH DATA: CFC TRANSPORT IN THE OCEAN

Principal Investigators: Rainer Bleck, EES-2
Synte Peacpock (formerly CNLS)

International efforts to observe the ocean are in high gear, given the prospect of rapid climate change triggered by oceanic circulation changes. Ocean models are evolving as well. A recent addition to the ocean model "gene pool" are the layer models, which, in contrast to tried-and-true *x, y, z* models, feature a quasi-material vertical coordinate. This coordinate substantially reduces inadvertent vertical mixing—the nemesis of ocean models used in decade-to-century climate prediction.

Efforts to combine the advantages of *x, y, z* and material coordinate models have led to the *hybrid model*, whose coordinate surfaces follow potential-density surfaces in the ocean interior but turn horizontal near the ocean surface. The hybrid coordinate concept resembles, but goes beyond, the LANL-developed ALE (Alternate Lagrangian-Eulerian) technique.

As part of a long-term effort to detect (and fix) biases in layered and hybrid ocean models, we test here the ability of a pure density coordinate model (Miami Isopycnic Coordinate Ocean Model [MICOM]) and a hybrid model (hybrid version of MICOM [HYCOM]) to reproduce the rate of chlorofluorocarbon-11 (CFC-11) penetration in the Indian Ocean against observational evidence.

External Reviews: None

Collaborators: None

Publications: None

#5 AQUEOUS ENVIRONMENTAL GEOCHEMISTRY OF MORTANDAD CANYON

Principal Investigators: Patrick Longmire, EES-6
Dale Counce, EES-6
Brent Newman, EES-2

Los Alamos National Laboratory's Environmental Restoration Project is conducting aqueous geochemical investigations in Mortandad Canyon to determine the extent of contamination in both the vadose zone, including perched groundwater, and the regional aquifer. These investigations use the integration of environmental chemistry, earth sciences, and computations to quantify contaminant transport in the subsurface.

The most significant contaminants observed at LANL are found in both groundwater and in the unsaturated zone beneath Mortandad. This significance is based on the variety and volume of mobile and adsorbing solutes discharged into the canyon and the canyon's proximity to a supply well Pajarito Mesa (PM)-5. Laboratory surveillance data collected for ephemeral surface water and alluvial groundwater in Mortandad Canyon show elevated concentrations or activities of ClO_4^-, NO_3^-, ^3H, $^{90}Sr^{2+}$, $^{238,239,240}Pu(IV, V)$, $^{137}Cs^+$, $^{241}Am(III)$, $^{234,235,238}U(VI)$, trace solutes, and major ions. Concentrations of NO_3^- as high as 700 ppm have been observed in alluvial groundwater from 1971 through 1984.

Four characterization wells and one borehole were recently installed to investigate the nature and extent of contamination in deep-perched groundwater and the regional aquifer. Investigation boreholes were installed to depths of 743 to 1325 ft by a combination of hollow-stem auger and fluid-assisted air-rotary methods. The distribution of contaminants in the vadose zone was characterized by analyzing radionuclides, metals, and anions present in core samples and in moisture extracted from the samples. Saturated zones were characterized by analyzing groundwater collected from developed wells and the borehole during drilling.

Analytes of interest include actinides, fission products, ^3H, ClO_4^-, NO_3^-, stable isotopes of hydrogen, nitrogen, and oxygen, major ions, iron, manganese, and other trace solutes. Sources of ClO_4^- and NO_3^- include neutralized perchloric acid and nitric acid, respectively. Recently, concentrations of these two anions and other radionuclides have significantly decreased within the treated effluent discharged to Mortandad Canyon.

The unsaturated zone was characterized by conducting leach experiments using deionized water on numerous core samples. Leachate solutions contained significant activities or concentrations of ^3H, ClO_4^-, NO_3^-, and other anions. The most mobile solutes included ^3H, ClO_4^-, and NO_3^-. Perchlorate is a recalcitrant anion stable under oxidizing conditions. The overall half-cell reaction for the ClO_4^-/Cl^- redox couple is given by:

$$ClO_4^- + 8H^+ + 8e^- \rightarrow Cl^- + 4H_2O \text{ and } Eh\ (V) = 1.39 - 0.0592pH.$$

Anaerobic conditions characterized by nitrate and sulfate reduction are required for reducing ClO_4^- to Cl^- as a result of the strong stability of this tetrahedrally coordinated molecule. Oxidizing conditions dominate, however, in the vadose zone beneath Mortandad Canyon; it is very likely that ClO_4^- will persist in the environment for long periods of time.

The U.S. Environmental Protection Agency (EPA) recently proposed a calculated risk level for ClO_4^- in drinking water at 1 ppb. Concentrations of ClO_4^- and NO_3^- measured in this perched zone were 142 ppb and 13.2 ppm, respectively. Concentrations of ClO_4^- and NO_3^-

were in the hundreds of ppb and ppm, respectively, within the unsaturated zone at depths of 400 ft or less. Activities of ^{3}H as high as 14,900 pCi/L have been observed in perched groundwater at a depth of 524 ft beneath the canyon floor. Concentrations of ClO_4^- and NO_3^- measured in the regional aquifer were less than 4.2 ppb and 2.3 ppm, respectively, indicating the breakthrough of anthropogenic NO_3^-. Low activities of ^{3}H (< 4 pCi/L) within the regional aquifer at well R-15 suggest that most of the groundwater is greater than 60 years old and predated nuclear testing. Concentrations of dissolved uranium are less than 2 ppb within perched zones and the regional aquifer.

Results of $\delta^{15}N$ (NO_3) analyses of the leachate solutions and groundwater samples suggest that nitrate is derived from neutralized nitric acid discharges. Groundwater within the alluvium, Cerros del Rio basalt, and Puye Formation varies in $\delta^{15}N$ ratios suggesting that different types of fractionated NO_3^- were discharged to the canyon. Isotopically light NO_3^- (highly enriched ^{14}N) was discharged from TA-50 from 1986 through 1989, and has been traced to depths of 500 ft. This unique NO_3^- is possibly the lightest isotopic nitrogen that has been measured worldwide with $\delta^{15}N$ ratios as light as –115% within the unsaturated zone. Stable isotope ratios of δD and $\delta^{18}O$ imply that perched groundwater and the regional aquifer groundwater were derived from a local meteoric source, consisting of precipitation and surface water.

In assessing groundwater chemistry and refining the geochemical conceptual model for Mortandad Canyon, we performed geochemical calculations using the computer program MINTEQA2 to evaluate solute speciation and mineral equilibrium. Results suggest that the perched groundwater and the regional aquifer is in close equilibrium with amorphous silica phases or volcanic glass and is undersaturated with respect to $CaCO_3$ and $SrCO_3$. This suggests that the mobility of $^{90}Sr^{2+}$ is controlled by cation exchange rather than mineral equilibrium. Major cations and anions are calculated to occur as free or uncomplexed solutes. Alkalinity (HCO_3^-) provides ligands for complexing with uranium(VI). Uranium(VI) is calculated to be stable as $UO_2(CO_3)_2^{2-}$ and $UO_2(CO_3)_3^{4-}$ complexes under oxidizing conditions. Calculation results agree with observed mineralogy and groundwater analytical results.

External Reviews: None

Collaborators: None

Publications:

Longmire, P., “Characterization Well R-15,” Los Alamos National Laboratory report LA-13896-MS (March 2002).

Broxton, D., et al., “Characterization Well MCOBT-4.4 and Borehole MCOBT-8.5 Completion Report,” Los Alamos National Laboratory report LA-13993-MS (December 2002).

Longmire, P., et al., “Characterization Well R-15 Completion Report,” Los Alamos National Laboratory report LA-13749-MS (May 2001).

#6 GROUNDWATER PATHWAY ANALYSIS FOR THE PAJARITO PLATEAU

Principal Investigators: Kay Birdsell, EES-6
Diana Hollis, RRES-SA
Brent Newman, EES-2

Co-Investigators: Velimir Vesselinov, EES-6
Paul Davis, Contract
Marc Witkowski, EES-9
Ed Kwicklis, EES-6

The groundwater pathway analysis for the Pajarito Plateau prioritizes LANL-contaminated sites based on their potential risks to groundwater receptors. The analysis evaluates the adequacy of the existing groundwater-monitoring network in terms of groundwater protection. EES Division's contribution to this project has several components: (1) screening to identify high priority sites, (2) quantification of source-term, (3) simulations of vadose-zone transport, and (4) simulations of regional aquifer transport. The analysis links several models to predict contaminant migration from the source to a potential receptor. In particular, contaminant concentrations reaching water-supply wells are input to a risk-assessment model that predicts potential risk over the next 100 years. The analysis also estimates the likelihood that contaminants will be detected by regional monitoring wells prior to reaching water-supply wells. The EPA Region VI Corrective Action Strategy document defines our approach for risk assessment.

The screening method overlays contaminant maps onto a map of vadose-zone, groundwater travel-time predictions. Contaminated areas with vadose-zone travel times of 100 years or less require further analysis. This screening method identified watersheds in Mortandad Canyon, Los Alamos/Pueblo Canyons, Cañon de Valle/Water Canyons, Pajarito Canyon, and Sandia Canyon. Further analysis for Mortandad Canyon and Cañon de Valle/Water Canyon has begun.

This poster focuses on work in progress for Mortandad Canyon. A first-order bounding calculation found that a more detailed, probabilistic risk assessment is required to properly evaluate perchlorate migration from this canyon. The probabilistic approach will consider uncertainty in conceptual models, source term, infiltration rates, hydrologic properties, and other site and model parameters. This approach will provide realistic estimates, including uncertainty bounds, of potential groundwater risk from the site. It should also identify the most important conceptual models and parameters controlling groundwater risk. Such information can then be used to guide further site characterization activities, identify potential corrective actions, and/or determine monitoring requirements.

External Reviews: External Advisory Group to the LANL Groundwater Integration Team

Collaborators:	David Rogers, RRES-WQH Elizabeth Keating, EES-6 Bruce Robinson, EES-6 Martin Nilsson, EES-6 Chris Echohawk, EES-9 Pat Longmire, EES-6 Leslie Dale, Contract Greg Cole, EES-6 Bill Carey, EES-6
Publications:	None

#7 TRACING ENVIRONMENTAL PROCESSES AT LANL USING STABLE ISOTOPES

Principal Investigator: Jeffrey Heikoop, EES-6

Co-Investigators: Julianna Fessenden-Rahn, EES-6
Donald Hickmott, EES-6

We are using light stable isotopes to identify ecologic processes relevant to issues of natural attenuation of contaminants in riparian and wetland settings at Los Alamos National Laboratory. Nitrogen isotopes were used to identify the occurrence of microbial denitrification in wetlands in Sandia Canyon (TA-60), Martin Canyon (TA-11), and Cañon de Valle (TA-16). Denitrification is a process in which microbes reduce nitrate to nitrogen gas under oxygen-poor conditions, resulting in the release of nitrogen from sediments.

The Sandia Canyon wetland receives treated sewage effluent from the Laboratory. This effluent contains nitrate highly enriched in the heavy isotope of nitrogen, ^{15}N, with a $d^{15}N$ of 32.4%. The delta notation is the ratio of $^{15}N/^{14}N$ relative to an international standard and expressed as parts per thousand or per mille. Cattail stems from the wetlands were measured for $d^{15}N$. Cattails near the head of the wetlands have values up to nearly 38%, the highest values for plants of which we are aware.

Denitrification is a fractionating process in which the residual nitrate available for plant uptake is progressively enriched in ^{15}N. The high $d^{15}N$ values for the cattails, relative to the value of input sewage nitrate, as well as trends towards higher $d^{15}N$ in more oxygen-depleted sediments, indicate that denitrification is an important natural attenuation process in the Sandia wetlands (Heikoop, et al., 2002). Cattail carbon isotope variation in the wetlands is related to redox conditions in the marsh. Redox stress in cattails mimics water stress such that cattails growing in more oxygen-depleted sediments are enriched in the heavy isotope of carbon, ^{13}C.

In Martin Canyon and Cañon de Valle, the nitrogen-bearing contaminants are nitrate and high explosives associated with the production of barium nitrate, RDX, and HMX at TA-16. While the value of $d^{15}N$ of the explosives is unknown, we know that the value must be close to 0% because nitric acid is used in their production and typically has a value near zero. Despite the input of isotopically light nitrogen, grasses and cattails associated with wetlands and springs have enriched values up to nearly 12%, again suggesting that denitrification is an important natural attenuation process.

These studies were designed to develop a quick, cost-effective technique to map the spatial variability in processes that can naturally attenuate contaminants without the need for application of expensive, invasive cleanup technologies. This research was funded as part of a postdoctoral fellowship to Jeffrey M. Heikoop and as part of the Laboratory Environmental Restoration Project.

External Reviews: None

Collaborators: None

Publications: Heikoop, J.M., et al., “N-15 Signals of Nitrogen Source and Fate in a Semi-Arid Wetland,” in *Wetlands and Remediation II*., Nehring K.W. and Brauning, S.E., Eds. (Battelle Press, Columbus, Ohio, 2002) pp. 355–362.

#8 NUMERICAL MODELING OF NAPL SOURCE ZONE TREATMENT USING LANL'S ASCI Q SUPERCOMPUTER

LA-UR 02-7843

Principal Investigators: Peter Lichtner, EES-6

Co-Investigators: Glenn Hammond, UILUC-DOE Computation Science Graduate Fellow
Albert Valocchi, UILUC

Over the past two years, we have developed the parallel multicomponent reactive transport code PARTRAN, which is founded upon the powerful PETSc library for parallel computing developed at Argonne National Laboratory (Balay, et al., 2002). The code has exhibited exceptional scalability on Theta, Lambda, and ASCI Q (Hammond, et al., 2001; Hammond, et al., 2002a, b). Features of the code include implementation of novel preconditioning and solver algorithms developed at LANL, such as the Jacobian-free Newton-Krylov with physics-based preconditioning (Mousseau, et al., 2000). The code is portable to any platform on which PETSc will run, resulting in near platform independence. Currently, the code has been compiled and run on HP/Compaq Alpha (ASCI Q, 1024 processors), SGI Origin 2000 (Theta, 128 processors), Linux clusters (Lambda, 1164 processors), multiprocessor Solaris (4 processors), and dual processor Mac OS X and Windows platforms.

Recently, PARTRAN was applied to analyze biogeochemical processes involved in reductive dehalogenation of chlorinated solvents associated with in situ bioremediation of contaminated superfund sites (Hammond, et al., 2002b). The code was run on LANL's ASCI Q machine with 512 processors. Reactions included mineral precipitation/dissolution, NAPL (nonaqueous phase liquid) dissolution, NAPL sorption, ion exchange, aqueous complexation, and biodegradation. The calculation involved a heterogeneous flow domain 60 m × 40 m × 10 m discretized on a grid with 120, 80, and 80 nodes in the x-, y- and z-directions, respectively, totaling 768,000 spatial degrees of freedom. In addition, 28 chemical components are used, giving a total of 21,504,000 degrees of freedom. The calculation required 90 GB of RAM and took 3.35 h to complete.

External Reviews: None

Collaborators: Vince Mousseau, T-3
Dana Knoll, T-3

Publications:

Hammond, G.E., et al., "An Evaluation of the Jacobian-Free Newton-Krylov Algorithm Applied to Multicomponent Reactive Transport Problems Using Parallel Computing" (SIAM Conference on Mathematical and Computational Issues in the Geosciences, Boulder, CO, June 11-14, 2001).

Hammond, G.E., et al., "Modeling Multicomponent Reactive Transport on Parallel Computers Using Jacobian-Free Newton-Krylov with Operator-Split Preconditioning" *Developments in Water Science* **1**, 727–734 (2002).

Hammond, G.E., et al., "Numerical Modeling of NAPL Source Zone Treatment," in *American Geophysical Union Fall Meeting Abstracts* (San Francisco, CA, December 6–10, 2002) p. 202.

#9 COLLOID-FACILITATED TRANSPORT IN FRACTURED ROCKS: PARAMETER ESTIMATION AND COMPARISON WITH EXPERIMENTAL DATA

Principal Investigators: Hari S. Viswanathan, EES-6, LANL
Andrew V. Wolfsberg, EES-6, LANL

Co Investigators: Paul W. Reimus, C-INC
Doug Ware, C-INC
Guoping Lu, Lawrence Berkeley Laboratory

Colloid-facilitated migration of plutonium in fractured rock has been implicated in both field and laboratory studies. Other reactive radionuclides may also experience enhanced mobility due to groundwater colloids. Model prediction of this process is necessary for assessment of contaminant boundaries in systems for which radionuclides are already in the groundwater and for performance assessment of potential repositories for radioactive waste. Therefore, a reactive transport model is developed and parameterized using results from controlled laboratory fracture column experiments.

Silica, montmorillonite and clinoptilolite colloids are used in the experiments along with plutonium and Tritium.. The goal of the numerical model is to identify and parameterize the physical and chemical processes that affect the colloid-facilitated transport of plutonium in the fractures. The parameters used in this model are similar in form to those that might be used in a field-scale transport model.

External Reviews: None

Collaborators: None

Publications: Viswanathan, H.S., A.V. Wolfsberg, P.W. Reimus, D. Ware, and G. Lu, Colloid-Facilitated Transport in Fractured Rocks: Parameter Estimation and Comparison with Experimental Data, Proceedings of the International High-Level Waste Conference, Las Vegas, March 30-April 2, 2003.

#10 SUBSURFACE GEOLOGICAL CHARACTERIZATIONS AT FRENCHMAN AND YUCCA FLATS, NEVADA TEST SITE: IMPLICATIONS TO HYDROGEOLOGIC INVESTIGATIONS

Principal Investigator: Giday WoldeGabriel, EES-6

Co-Investigators: Steve Chipera, EES-2
Gordon Keating, EES-2
Emily Kluk, EES-2
Schon Levy, EES-2
Peg Snow, EES-2

The Frenchman and Yucca Flats located along the eastern part of the Nevada Test Site (NTS) are major hydrologically closed north-south-trending Cenozoic basins, which formed as a result of basin-and-range extensional tectonics. Both basins currently contain seasonal playas in their respective topographic lows. Both basins were extensively used during the nation's underground nuclear weapons testing program. Approximately a third of these tests occurred near or below the water table, resulting in some radioactive contamination of the groundwater. A Hydrologic Investigation Well Program in the area of Frenchman and Yucca Flats was implemented as part of the NNSA/NV Environmental Restoration Project at the NTS. The proposed program's goal is to identify the location of radiological risks in groundwater, predict the movement of potentially contaminated groundwater, define the extent of migration, and establish long-term monitoring systems. As part of this program, seven deep and medium wells were drilled in the central part of Frenchman Flats and at several important locations within Yucca Flats where most of the underground testing was conducted.

Understanding the subsurface geology and hydrogeology of the NTS is key to accomplishing the scientific objectives mentioned above. The subsurface studies are aimed at completing the following tasks: (1) identifying the major subsurface stratigraphic and hydrostratigraphic units and associated alteration mineral assemblages, (2) characterizing geologic structures, (3) providing hydrologic parameters and source-term data, (4) determining hydraulic properties of hydrostratigraphic units, (5) providing water-level data and assessing groundwater flow systems within each basin, (6) collecting and analyzing groundwater for contaminants, (7) using wells for long-term monitoring points, and (8) ultimately developing and validating 3-D hydrogeological framework models. Equipped with these objectives and guidelines, we drilled two of the wells in the central part of Frenchman Flats.

The 3732-ft deep ER-5-4 and the 7000-ft deep ER-5-4 #2 were drilled 100 ft apart within a cluster of other shallow drill holes. ER-5-4 ended within the alluvium, whereas ER-5-4 #2 penetrated to the base of the Tertiary volcanic sequence. At least 12 distinctive alluvial layers dominated by volcanic clasts embedded within vitric matrix were described in ER-5-4. Smectite, zeolites, calcite, and secondary silica were present within the alluvial layers; however, there was very little evidence for post-depositional alteration as indicated by the primarily vitric matrix of the alluvium. Although the secondary minerals represent relatively high reactive surfaces, the clays coat other primary and secondary reactive minerals. Unlike the alluvium of ER-5-4, volcanic rocks characterized by pervasive alteration dominated the lower half of ER5-4 #2. Abundant smectite, clinoptilolite, mordenite, silica, and calcite in ER-5-4 #2 provided relatively high reaction surfaces and have the potential of reducing permeability of the host rocks.

Abundant subsurface data was available from underground testing locations in Yucca Flat. However, the regions outside these areas are poorly characterized. Five wells were drilled at the northern, east central, and southeastern parts of the area down-gradient from underground test sites. The drill holes penetrated the volcanic sequence into the Paleozoic rocks. Complete geological characterization is in progress on cuttings from the five Yucca Flats wells, like the ER-5-4 and ER-5-4 #2 wells of Frenchman Flats.

External Reviews:	None
Collaborators:	Sig Drellack, Bechtel Nevada Lance Prothro, Bechtel Nevada Jeff Wurtz, Shaw E&I
Publications:	None

#11 CARBON ANALYSIS IN SOILS AND TERRESTRIAL SEQUESTRATION BOLD IN CAPS

Principal Investigators: Michael H. Ebinger, EES-2
David D. Breshears, EES-2

Co-Investigators: David A. Cremers, C-ADI
Pat J. Unkefer, B-3

Terrestrial carbon fluxes account for more than half of the carbon transferred between land and atmosphere. The amount of carbon that could be sequestered terrestrially is potentially large but controversial. Even if we cannot sequester large amounts of carbon, there are important benefits and liabilities that must be considered. The benefits include improving productivity of carbon-depleted lands by increasing soil quality. Liabilities that should be considered are the large and rapid losses of carbon, such as during erosion caused by fire and drought that release carbon from soils and further degrade the land.

To manage carbon, we must be able to account for it by measurement and/or modeling. Our work addresses a variety of issues relative to improved carbon measurement and management, including (1) the development and demonstration of advanced soil carbon measurement using Laser-Induced Breakdown Spectroscopy (LIBS); (2) the measurement of soil carbon inventory and dynamics as related to herbaceous and woody plants in semiarid ecosystems, including the potential for rapid carbon losses due to disturbances such as fire, drought, and associated increases in associated erosion; and (3) the evaluation of spatial and temporal variation in water balance dynamics as drivers for carbon dynamics.

Using LIBS, we analyzed total soil carbon at spatial resolution of 1 mm to 1 cm in soil profiles. Our LIBS data show significant variation in carbon concentrations with respect to depth; and the variation is correlated with various soil properties. LIBS measurements from intact soil cores were calibrated using dry combustion of the same soil cores to ensure comparability between LIBS data and conventional carbon data. Carbon data from 1 m soil cores can be extracted in less than 1 hour with this method and at significant cost savings resulting from reduced sample preparation and analysis time.

Soil carbon inventories show that woody plants in a semiarid piñon-juniper woodland do not greatly affect soil carbon inventories. The soil patches beneath woody canopies have more soil carbon than soils in intercanopies, particularly at shallow depths. Neither tree species nor size has much effect on these inventories. These data, in concert with other recent studies, suggest that woody plant encroachment may account for less of the missing carbon than previously assumed and that options for terrestrial sequestration are more limited.

Our work on soil water drivers has yielded patterns of soil water availability based on a 15-year data set, perhaps the longest data set of its kind. The results highlight how the amount of water available to plants varies between “wet vs. dry years,” “snow- vs. rain-dominated months,” and spatially, both vertically and horizontally. These soil water dynamics are a key driver of carbon dynamics of woody and herbaceous plants.

External Reviews: National Energy Technology Laboratory External Panel, February 2002. LIBS Ranked first of three projects in terrestrial carbon sequestration.

Collaborators:

Craig D. Allen, U.S. Geological Survey
M. L. Norfleet, USDA
Bradford P. Wilcox, Texas A&M University
Paul W. Zedler, University of Wisconsin, Madison

Publications:

Ebinger, M.H., et al., "Extending the Applicability of Laser-Induced Breakdown Spectroscopy for Total Soil Carbon Measurement" (to be published in *Soil Sci. Soc. Am. J.*).

Wilcox, B.P., et al., "Hydraulic Conductivity in a Piñon-Juniper Woodland: Influence of Vegetation" (to be published in *Soil Sci. Soc. Am. J.*).

House, J., et al., "Conundrums in Mixed Woody-Herbaceous Plant Systems" (to be published in *J. Biogeogr.*).

Wilcox, B.P., et al., "Ecohydrology of a Resource-Conserving Semiarid Woodland: Effects of Scale and Disturbance" (to be published in *Ecol. Monogr.*).

Breshears, D.D. et al., "The Importance of Rapid, Disturbance-Induced Losses in Carbon Management and Sequestration." *Global Ecology and Biogeography* **11**, 1-5 (2000).

#12 CO_2 INJECTION IN A DEPLETED OIL RESERVOIR IN HOBBS, NM

Principal Investigators: Rajesh Pawar, EES-6,
Dongxiao Zhang, EES-6

Carbon-dioxide sequestration in geologic formations is the most direct carbon management strategy for long-term removal of anthropogenic CO_2 from the atmosphere. It is likely to be needed for continuation of the U.S. fossil-fuel-based economy and high standard of living. Subsurface injection of CO_2 into depleted oil reservoirs is a carbon sequestration strategy that might prove to be both cost-effective and environmentally safe. In part, this is due to an extensive knowledge base about site-specific reservoir properties and subsurface gas-fluid-rock processes from the mining and petroleum industries, including those from recent Enhanced Oil Recovery (EOR) CO_2 flooding activities. However, CO_2 sequestration in oil reservoirs is a complex issue spanning a wide range of scientific, technological, economic, safety, and regulatory issues. Further understanding of these interactions is necessary before this option can become a safe and economical sequestration option; it requires a more focused R&D effort by government and private industry.

This paper provides an overview and update of our NETL (National Energy Technology Laboratory)-sponsored CO_2 sequestration project to predict and monitor the migration and ultimate fate of CO_2 after it is injected into a depleted oil reservoir. This project is a collaborative effort between Los Alamos National Laboratory, New Mexico Tech, Sandia National Laboratories, and Strata Production Company. The overall objective of our project is to better understand CO_2 sequestration processes in a depleted sandstone oil reservoir. The project combines geologic and flow/reaction modeling, injection of CO_2 into an oil-producing reservoir, geophysical monitoring of the advancing CO_2 plume, and laboratory experiments to measure reservoir changes with CO_2 flooding.

The computer and lab results, in conjunction with the micro-pilot-scale field experiment, will allow for a better understanding and prediction of complex geologic sequestration processes. An important milestone in the project was achieved on February 10, 2003, when injection of ~2000 tones of CO_2 was completed. At the time the injection was stopped and the injection well was shut off. Currently the reservoir is under a soak period. Geophysical surveys are planned to monitor injected CO_2 plume during the soaking period. Following the soak period, CO_2 will be vented out and fluid samples will be collected to determine changes in fluid composition. The field and laboratory data are currently being incorporated in numerical models.

External Reviews: NETL performed external reviews.

Collaborators: H. Westrich, Sandia National Laboratories
R. Grigg, New Mexico Institute of Mining and Technology
B. Stubbs, Strata

Publications: Krumhansl, J., et al., "Geological Sequestration of Carbon Dioxide in a Depleted Oil Reservoir" (The SPE/DOE Thirteenth Symposium on Improved Oil Recovery, Tulsa, Oklahoma, April 13–17, 2002).

Pawar, R.J. et al., “Sequestration of CO_2 in a Depleted Oil Reservoir: Numerical Simulations Related to a Field Demonstration” (International Pittsburgh Coal Conference, Newcastle, New South Wales, Australia, December 4–7, 2001).

Pawar, R.J., et al., “Sequestration of CO_2 in a Depleted Oil Reservoir: Preliminary Simulation Study” (The First National Carbon Sequestration Conference Proceedings, May 15–17, 2001).

#13 STOCHASTIC RESERVOIR SIMULATIONS

Principal Investigators: Dongxiao Zhang, EES-6
Zhiming Lu, EES-6

Accurately predicting oil/gas reserves requires detailed knowledge of the spatial description of reservoir properties, such as permeability and porosity. However, only limited reservoir characterization information of varying quality (from different sources) is usually available. Incomplete knowledge of the reservoir description leads to uncertainty in reservoir performance predictions obtained from numerical simulations.

The current industrial practice is to quantify such uncertainty using the method of Monte Carlo simulation, which is computationally expensive. The objective of our work is to develop alternative techniques and practical tools for directly quantifying the uncertainty in reservoir performance predictions. More specifically, we are developing a moment-equation-based approach to simulate single and multiphase flow in heterogeneous oil/gas reservoirs.

Our research includes mathematical derivation of moment equations from the original stochastic flow equations, numerical implementation of computational algorithms to solve these moment equations, and validation of the proposed approach by comparing with Monte Carlo simulations in both computational efforts and numerical results. We also demonstrate the applicability of the approach by applying it to real-world problems.

External Reviews: External Reviews by NETL, NGOTP (National Gas/Oil Technology Partnership).

Collaborators: Hamdi Tchelepi, Chevron Texaco
Liyong Li, Chevron Texaco

Publications:

Lu, Z. et al., "Solute Spreading in Nonstationary Flows in Bounded Heterogeneous Unsaturated—Saturated Media" (to be published in *Water Resour. Res.*).

Lu, Z., et al., "On Stochastic Study of Well Capture Zones in Bounded, Randomly Heterogeneous Media" (to be published in *Water Resour. Res.*).

Lu, Z., et al., "Stochastic Analysis of Transient Flow in Heterogeneous, Variably Saturated Porous Media: The van Genuchten-Mualem Constitutive Model," *Vadose Zone Journal* **1**, 137–149 (2002).

Lu, Z., et al., "On Stochastic Modeling of Flow in Multimodal Heterogeneous Formations, *Water Resour. Res.* **38**, 1190, doi:10.1029/2001WR001026 (2002).

Zhang, D., et al., "Stochastic Analysis of Flow in a Heterogeneous Unsaturated-Saturated System," *Water Resour. Res.* ***38***, 1018, doi:10.1029/2001WR000515 (2002).

#14 STUDIES OF THE CONSEQUENCES OF OCEAN CARBON SEQUESTRATION USING LOS ALAMOS MODELS

Principal Investigator: Shaoping Chu, EES-2

Co-Investigators: Scott Elliott, EES-2
Mathew Maltrud, T-3

Our research emphasizes fine resolution simulation of patch-scale ocean iron-fertilization exercises. We have recently developed a biogeochemical version of the Los Alamos Parallel Ocean Program (POP) that supports global scale runs at grid-cell sizes of one-fifth of a degree latitude/longitude. This model is being applied to the simulation of generic iron enrichment experiments, on the order of 30 square patches (100 kilometers on a side), distributed simultaneously over the North Pacific, equatorial regions, and the Southern Ocean.

We ran control and iron fertilization situations side by side and compared the resulting carbon flows and fluxes for all sites (i.e., air-sea, particulate sedimentation, dissolved and particulate pools). We were able to rank each location based on its dominant flux characteristics. Results were also compared with in situ experiments and analyzed against model trajectories and in situ drifters. The agreement between the simulations and our observations was reasonable. For example, several computed patches mimicked behavior observed during the Southern Ocean Iron (Fe) experiments (SOFeX).

We also performed deep tracer injection experiments representing CO_2 injection at eight distinct locations in the Pacific and Southern Ocean. Coarse resolution POP versions carried the tracers for a 100-year period and calculated percent return to the surface at key points in time. Regions were identified from which sequestered CO_2 might return to the surface rapidly. Through such studies, we are investigating the overall efficiency of large-scale ocean fertilization and its impact on marine ecosystems, chemistry, and climate-altering trace gases emissions.

External Reviews: Francisco Chavez, Montery Bay Aquarium Research Institute
Fei Chai, University of Maine

Collaborators: Francisco Chavez, Montery Bay Aquarium Research Institute
Fei Chai, University of Maine

Publications:

Chu, S., et al., “Global Eddy Permitting Simulations of Surface Ocean Nitrogen, Iron, Sulfur Cycling,” *Chemosphere* **50**, 223–235 (2003).

Elliott, S. et al., Comment on “Ocean Fertilization Experiments May Initiate a Large Scale Phytoplankton Bloom” (to be published in *Geophys. Res. Lett.*).

Chu, S., et al., “Ecodynamics of Multiple Southern Ocean Iron Enrichments Simulated in a Global, Eddy Permitting GCM” (submitted to *Geophys. Res. Lett.*).

#15 **NEUTRON SCATTERING AND THE NONLINEAR ACOUSTIC PROPERTIES OF ROCKS**

LA-UR 02-3902

Principal Investigators: T.W, Darling, MST-10
J.A. TenCate, EES-11

Co-Investigators: S. Vogel, LANSCE-12
T.E. Proffen, LANSCE-12

Although the mechanical properties of geomaterials (rocks) have been studied for many decades, the complexity, inhomogeneities, multiple phases, fluid content, interfaces, and lack of transparency have defied most experiments to resolve the microscopic behavior associated with a particular macroscopic observation. The origin of nonlinearity and hysteresis (end-point memory) evident in the macroscopic stress-strain curves of rocks is still unknown after some 30 years of research, and the puzzle increases with recent low strain results like slow dynamics [see, *Physics Today* 52, 30-35 (1999)] and hysteretic temperature dependence [*Geophys. Res. Lett.* 28, 2293-2296 (2001)]. Although models using statistical assemblies of generic hysteretic elements have developed to a degree where some good qualitative agreement has been reached, the link to the actual physical microscopic or atomic mechanism for hysteresis is still missing.

Neutron diffraction is one of a few experiments that can lead to an understanding of the atomic or microscopic effects that govern the properties of complex geomaterials. Neutrons can easily penetrate rocks [Geophys. Res. Lett., 28, 2105-2108, (2001)] and reveal properties of the bulk interior material (rather than the near-surface regions measurable, say, by X-rays). We are performing experiments with rocks on three beamlines at the Manuel Lujan Jr. Neutron Scattering Center at LANL, where the scattering data will be correlated with some of the large body of nonlinear acoustic data to determine which atomic-plane level constituents of the rocks are active in nonlinear processes. We will describe the neutron scattering and acoustic experiments carried out on marble and sandstone samples and present initial results.

External Reviews: LDRD Program Review

Collaborators: Sven Vogel and Thomas Proffen, LANL, LANSCE-12

Publications: Vogel, S., et al. "Investigation of the Deformation Behavior of Rocks by Neutron Diffraction," (2003 Annual Meeting of The Minerals, Metals, and Materials Society, San Diego, March, 2003).

#16 TECHNICAL PROGRESS IN THE DEVELOPMENT OF ZERO EMISSION COAL TECHNOLOGIES

LA–UR 02–5969

Principal Investigator: H.J. Ziock, EES-6

Co-Investigators: T.W. Robison, C-ACT
B.F. Smith, C-ACT
B. Roop, C-SIC
G.D. Guthrie, EES-6
W. Parkinson, ESA-EPA
E.L. Brosha, MST-11
F.H. Garzon, MST-11
R. Mukundan, MST-11
K.S. Lackner, Columbia University
A.A. Johnson, ZECA Corporation
M. Nawaz, Nexant, Inc.
J. Ruby, Nexant, Inc.
A. Kramer, Gas Technology Institute
F. Lau, Gas Technology Institute
E.J. Anthony, CETC, Natural Resources Canada
J. Wang, CETC, Natural Resources Canada

We present an update on the development of technologies required for the Zero Emission Carbon (ZEC) concept being pursued by ZECA Corporation. The concept has a highly integrated design involving hydrogasification, a calcium oxide-driven reforming step that includes simultaneous CO_2 separation, coal-compatible fuel cells for electricity production and heat recovery, and a closed-loop gas system in which coal contaminants are removed either as liquids or solids. The process does not involve any combustion and, therefore, has no smokestack or air emissions.

An independent assessment of the concept by Nexant (a Bechtel-affiliated company) suggests a net efficiency of approximately 70% for the conversion of the higher heat value-(HHV) fuel energy into electrical output. This is even after the penalties of CO_2separation and pressurization to 1000 psi are taken into account. For CO_2sequestration, a variety of options are being considered, which include enhanced oil recovery in the near-term and mineral carbonation in the long-term.

We report on our early results in the development of sulfur-tolerant anode materials for solid oxide fuel cells, a critical analysis of the calcium oxide–calcium carbonate cycle, trace element removal, and the recent results of hydrogasification tests.

External Reviews: LDRD Program Review

Collaborators: See Author List

Publications: Several publications in Conference Proceedings.

#17 PREPARING FOR A HYDROGEN ECONOMY: SOURCES, SINKS, AND ENVIRONMENTAL IMPACTS

Principal Investigator: Thom Rahn, EES-6

Co Investigator: M. Dubey, EES-6

Molecular hydrogen (H_2) is the proposed basis for fuel-cell technologies anticipated to expand substantially in the coming decades. The atmospheric consequences of new anthropogenic sources of H_2 are not easily anticipated but may include effects such as increases in tropospheric ozone stratospheric water with the potential impact on atmospheric chemistry and the Earth's radiation budget. Preparation for such potential change must begin with a precise and accurate description of the contemporary budget. Currently, after methane, H_2, with an average concentration of ~500 ppb, is the second most abundant reduced gas in the atmosphere.

Long-term records of hydrogen concentration yield conflicting evidence as to the trend of average H_2 concentration. As has been shown with other important trace gases (e.g. carbon dioxide, methane, nitrous oxide), the stable isotopic (deuterium [D]) content of H_2 holds potential for refining our understanding of its sources and sinks. We have developed a new method for analysis of D in H_2 that reduces by three orders of magnitude the sample size required for atmospheric measurements. The reduction of sample size and consequent increase in sample throughput has enabled us to vastly expand our knowledge of the variability of D in H_2. Examples will be presented from environments ranging from urban basins to the stratosphere and from sources as diverse as automotive exhaust to captive termites.

External Reviews: None

Collaborators:
John Eiler, California Institute of Technology
Jim Randerson, California Institute of Technology
Paul Wennberg, California Institute of Technology
Jared Leadbetter, California Institute of Technology
Elliot Atlas, National Center for Atmospheric Research
Kristie Boering, University of California, Berkeley

Publications:

Rahn, T., et al., "D/H Ratios of Atmospheric H_2 in Urban Air: Results Using New Methods for Analysis of Nanomolar H2 Samples,"*Geochim. Cosmochim. Acta.* **66**, 2475–2481 (2002).

Rahn, T., et al., "Soil Uptake of H_2 in Boreal Forests: D/H Ratios and Relationship to Respiration," *Geophy. Res. Lett.* 2002GL015118 (2002).

Rahn, T., et al., "Extreme Deuterium Enrichment in Stratospheric H_2" (submitted to *Nature*).

#18 ON DYNAMIC NONLINEAR ELASTICITY AND SMALL STRAIN

Principal Investigators: Paul Johnson, EES-11
James TenCate, EES-11
Donatella Pasqualini, EES-11

Co Investigator: Robert Guyer, Dept. Physics, University of Massachusetts, Amherst

Numerous elastic wave measurements in diverse solids have established that rock, concrete, some metals, and damaged materials exhibit nonclassical, nonlinear behavior. By nonclassical behavior, we mean that a perturbation expansion of the stress-strain relation (the classical atomic-elastic approach used for anharmonicity by Landau and Lifshitz does not quantitatively predict observations). In dynamics, we say these materials exhibit anomalous fast nonlinear dynamics (ANFD) in that their elastic nonlinearity exhibits unique "signatures" not present in classical nonlinear wave dynamics. These "signatures" include highly nonlinear behavior; the scaling relations between driving strains and detected wave harmonics are unique, as is the relation of resonance-peak shift and change in specific dissipation as a function of driving strain. These materials are also known as nonlinear mesoscopic elastic (NME) materials because their elasticity is attributable to the ensemble elastic behavior within the "bond system" at scales that may be near molecular up to 6 to 10 meters.

We are currently addressing the question of whether or not there is a threshold strain behavior in rock and other solids, or if the nonlinearity persists to the smallest measurable values. In qualitative measures of many rock types and other materials that behave in the same manner, we have do not observe a threshold; however, the only careful, small-strain study conducted under controlled conditions that we are aware of is that of TenCate, et al. (2000) in Berea sandstone. This work indicated that in Berea Sandstone, the elastic nonlinearity persists to the minimum measured strains of less than 10^{-7}. Recently, we have begun controlled experiments in other materials that exhibit nonclassical nonlinearity in order to see whether or not they behave as Berea sandstone does. In the more recent experimental configuration, strains of 10^{-8} can be recorded (an order of magnitude better than the 2000 experiments). The measurements are a surprise. There appears to be a threshold of elastic nonlinearity in some materials measured (e.g., Berea sandstone, Alumina ceramic, Meule sandstone), and the threshold is material-dependent. In some materials, there is no measurable threshold (e.g., Fontainbleau, pure quartz sandstone). However, based on our recent experience with Berea sandstone, a threshold likely exists, but we do not yet have the means to measure it. In this (these) materials(s), a gradual transition from hysteretic (nonclassical) to some other type of elastic nonlinearity may take place eventually leading to linear elastic behavior.

Strain threshold behavior is important to understanding the origin of elastic nonlinear behavior, which is currently a mystery. In our current thinking, frequency shift translates to the ensemble response of a sufficient number of atomic potential energy barrier hopping, creating an observable net softening of the solid. The strain at which this occurs is proportional to the energy required to hop the barrier. The results indicate that barrier hopping takes place at the lowest measurable strains in Fontainbleau sandstone, translating to a spectrum of barrier potential energies. However, in alumina for instance, a minimum strain of approximately 2×10^{-7} is required, indicating that there may be some minimum barrier energy level. The fact that the strain threshold is material dependent could potentially be used as a diagnostic characteristic. An interesting corollary question should be addressed as well: in all materials studied, there is a different threshold level for slow dynamics than for material softening from an elastic wave. Why is that the case, and how are these phenomena related?

External Reviews: None

Collaborators: Salman Habib, Katrin Heitmann (post doc) T-7

Publications:

Johnson, P., et al., "Dynamic Measurements of the Nonlinear-Elastic Hysteretic Parameter a in Rock Under Varying Conditions" (submitted to *J. Geophys. Res.*).

Johnson, P. et al., "Slow Dynamics in Diverse Solids" (submitted to *Phys. Rev. B.*).

Lacouture, J.C. et al., "Study of Critical Behavior in Concrete During Curing by Application of Dynamic Linear and Nonlinear Means" (to be published in *J. Acoust. Soc.*).

Delsanto, P. et al., "Lisa Simulations of Time Reversed Acoustic and Elastic Wave Experiments" (to be published in *J. Phys. D*).

Scalerandi, M. et al., "Modeling of Nonclassical, Nonlinear Elastic Behavior in Materials" (to published in *J. Acoust. Soc. Am.*).

Ostrovsky, L. et al., "Nonlinear Dynamics of Rock: Hysteretic Behaviour" (to be published in *The Russian Academy of Sciences Journal on Acoustics*).

Van Den Abeele, K., et al., "The Influence of Water Saturation on the Nonlinear Mesoscopic Response of Earth Materials, and the Implications to the Mechanism of Nonlinearity," *J. Geophys. Res.* **107**, 1040 (2002).

Kazakov, V.V., et al., Sensitive Imaging of an Elastic Nonlinear Wave Source in a Solid, *Appl. Phys. Lett.* **81**, 646-648 (2002).

#19 WAVE PROPAGATION IN THE HETEROGENEOUS EARTH

Principal Investigator: Michael Fehler, EES-11

Co Investigator: Lianjie Huang, EES-11

High-frequency (>1Hz) seismograms are not only composed of direct P and S waves but also many waves scattered from heterogeneities distributed within the Earth that cannot be readily explained using deterministic models. Recognizing this complexity, seismologists use statistical characterization of the random heterogeneity, focusing on envelopes of band-pass filtered traces that disregard phase information (e.g., Sato and Fehler, 1998).

For the stochastic study of the Earth's medium heterogeneity using seismic signals, it is useful to measure how coda envelopes decay with increasing lapse time and seismogram envelopes collapse with increasing travel distance. The spectra of medium heterogeneity have been found from two approaches, which focus independently on either the frequency dependence of coda excitation or envelope broadening. Coda excitation provides information about medium heterogeneity by using the radiative transfer theory with scattering amplitude predicted with the Born approximation. Envelope broadening around the direct arrival is predicted by using the Markov approximation. In general, forward scattering dominates at large wave numbers, and the multiple forward scattering process is well described by the parabolic wave equation. The Markov approximation is a stochastic treatment of the parabolic wave equation for the second moment of wave fields.

In order to explain the whole envelope starting from onset to coda, we have proposed a preliminary model (Saito, et al., 2002), in which the direct propagation term, written as a delta function in the conventional solution of the radiative transfer equation for isotropic scattering case, is replaced with the Markov envelope that has a finite time width. We have validated this model by comparing it with simulations for an ensemble of random media and found it works well in many cases. More recently, we have developed a method in which the envelope calculated using the Markov approach is used as a propagator in the radiative transfer theory. This allows for a more complete accounting of forward scattering by the modified radiative transfer theory model.

In addition, we have been using results of numerical simulations to investigate how the spatial variation in recorded seismic wavefield can be used to determine the spatial characteristics of the random media. We have found that the integral of the rectified seismic trace has spatial spectral characteristics that are similar to those of the random media. This provides a potentially valuable new tool for characterizing the statistical structure of the random portion of the Earth's velocity field.

External Reviews: Part of peer-reviewed proposal submitted to DOE/OBES in 2000.

Collaborators: Haruo Sato, Department of Geophysics, Graduate School of Science, Tohoku University
Tatsushiko Saito, Department of Geophysics, Graduate School of Science, Tohoku University
Masakazu Ohtake, Department of Geophysics, Graduate School of Science, Tohoku University
Ru-Shan Wu, Modeling and Imaging Laboratory, University of California at Santa Cruz

Publications:

Sato, H., et al., *Seismic Wave Propagation and Scattering in the Heterogeneous Earth* (Springer-Verlag & American Institute of Physics Press, 1998).

Fehler, M., et al., "Envelope Broadening of Outgoing Waves in 2-D Random Media: A Comparison Between the Markov Approximation and Numerical Simulations," *Bull. Seismol. Soc. Am.* **90**, 914–928 (2000).

Sato, H., et al., "Scattering and Attenuation of Seismic Waves in the Lithosphere," in *International Handbook of Earthquake and Engineering Seismology*, P Jennings, H. Kanamori, and W. Lee, Eds. (Academic Press, 2002) pp. 195–208.

Fehler, M. et al., "Coda," *Pure Appl. Geophys.* **160**, 541–554 (2003).

Saito, T., et al., "Simulating the Envelope of Scaler Waves in 2-D Random Media having Power-Law Spectra of Velocity Fluctuation" (to be published in *Bull. Seism. Soc. Am.*).

Pride, S, et al., "Permeability dependence of seismic Amplitudes" (to be published in *The Leading Edge*).

#20 VERTICAL TRANSPORT AND MIXING IN THE STABLE BOUNDARY LAYER

Principal Investigator: Keeley Costigan, EES-2

The Salt Lake City basin was the location of the Vertical Transport and Mixing (VTMX) program field experiment in October 2000; it is an area that has experienced urban air quality problems. In addition to the known night-time drainage winds from canyons entering the valley from the east, most of the experiment's intensive observation periods (IOPs) found that air flow through the Jordan Narrows—the gap in the Traverse Range that divides the Salt Lake City basin from the Utah Lake basin to its south—was significant. Simulations of IOPs 7 and 8 with the Regional Atmospheric Modeling System (RAMS) have yielded results that suggest that synoptic weather conditions influence the timing and location of the interaction of the Jordan Narrows flow with canyon drainage flows. The relative strength and locations of these vertical motions can lead to vertical transport and mixing.

Although the large-scale weather was relatively weak during both IOPs, the rawinsonde soundings from the airport indicate that the low-level vertical temperature gradient was more stable during IOP 7, and the winds above ridge top were light and from the east. In contrast, the ridge-top winds during IOP 8 were somewhat stronger and from the west. Lidar and surface observations in the Salt Lake City basin indicate that the flow through the Jordan Narrows, from the south, begins earlier in the night and is stronger during IOP 7 than during IOP 8.

The model results agreed qualitatively with the observations by producing stronger and earlier down-valley (southerly) flow through the Jordan Narrows during IOP 7 than during IOP 8. The strength and timing of the canyon outflows were also different during the two IOPs, suggesting that they may also be influenced by ridge-top wind direction, which is defined by synoptic conditions and can reinforce or oppose the canyon drainage flows. The down-valley flow converges with the canyon outflows earlier in the simulation of IOP 7, producing localized areas of vertical motion in the Salt Lake City basin earlier in the evening. Prior to sunrise, both simulations showed down-valley flow in the basin converging with canyon outflows, but the locations of the associated vertical motions are somewhat different. The magnitudes are much larger for IOP 7. These simulations also indicate that the flow over the Traverse Mountains and through the Narrows generated a gravity wave. This gravity wave has higher amplitude and greater vertical motions during IOP 7.

External Reviews: None

Collaborators:: Bob Banta, NOAA ETL, Boulder, CO
Lisa Darby, NOAA ETL, Boulder, CO

Publications: None

#21 AN APATITE II PERMEABLE REACTIVE BARRIER TO REMEDIATE PB, ZN, CD, IN ACID MINE DRAINAGE AT SUCCESS MINE

Principal Investigator: James Conca, EES-12

Co Investigator: Judith Wright, PIMS NW, Inc.

Phosphate-Induced Metal Stabilization (PIMS) employs the reactive media—Apatite II—in a subsurface permeable reactive barrier (PRB) to treat groundwater containing elevated levels of zinc, lead, cadmium, sulfate, and nitrate at the Success tailings/waste-rock pile. The impacted groundwater is treated in situ before it enters the east fork of Ninemile Creek, a tributary to the Coeur d'Alene River. Laboratory feasibility studies demonstrated the greater effectiveness and lower cost of Apatite II relative to eight other reactive media.

As a result, Apatite II was selected for use in a voluntary non-time-critical CERCLA (Comprehensive Environmental Response, Compensation and Liability Act) removal action completed by the Silver Valley Natural Resource Trustees (SVNRT) at the Success Mine and Mill site in northern Idaho. The emplaced PRB has been operating successfully since January 2001 and has reduced the concentrations of cadmium and lead to below detection (2 mg/L or ppb), zinc to near background (about 100 mg/L or ppb), and sulfate and nitrate to below detection (50 mg/L or ppb). The PRB, filled with 100 tons of Apatite II (at $350 per ton), has been in operation for over two years and has removed over 6,000 lbs of Zn, both sorbed onto the Apatite II and as ZnS, over 100 lbs of Pb as pyromorphite and over 50 lbs of Cd. As a result of this success, a second barrier has been installed 10 miles away at the Nevada Stewart Adit.

External Reviews: Ken Rice, Parsons Engineering
Mick Apted, Monitor Scientific

Collaborators: Bryony Hansen, Golder Associates

Publications: Wright, J. et al., "PIMS: an Apatite II Permeable Reactive Barrier to Remediate Groundwater Containing Zn, Pb and Cd" (to be published in *Environ. Geosci.*).

#22 THE ACTINIDE CHEMISTRY AND REPOSITORY SCIENCE PROGRAM IN SUPPORT OF THE WASTE ISOLATION PILOT PLANT (WIPP)

LA-UR 02-4165
and LA-UR 384

Principal Investigato/: Jean-Francois Lucchini, EES-12

Co-Investigators: Andrzej Rafalski, EES-12
James Conca, EES-12
Ningping Lu, C-Division

WIPP is a nuclear waste repository for the disposal of transuranic (TRU) waste located in a deep geological salt formation near Carlsbad, NM. Because of geochemical interactions expected in WIPP, corrosion and destruction can be expected in the long-term, which can cause actinide release into the environment. The Actinide Chemistry and Repository Science Program objectives are (1) to study the behavior of actinides (Pu, U) in the WIPP environment, and (2) to provide, through experimental studies, sufficient understanding of the chemistry of the repository environment.

The poster briefly exposes the current three axes of study: (1) actinide chemistry in brine solutions, (2) brine radiolysis, and (3) analytical technique and method development.

We are studying the oxidation state, speciation, and solubility of the actinide elements U and Pu in high ionic strength brine solutions representative of radioactive waste repositories located in geologic salt deposits. These properties have and will be studied in the presence of major radiolytic byproducts such as hydrogen peroxide (H_2O_2) and hypochlorite (OCl-), as well as in the presence of major reducing agents (Fe, Al) that come from the containers, and, finally, in the presence of the MgO backfill material that is emplaced around the waste. Previous results show that the MgO backfill sequesters Pu (VI) from WIPP brines as Pu (IV) on its surface.

Also of interest is brine radiolysis because radiolysis is expected to become the driving force in the redox potential modification in brines. Ion beam line experiments confirm the hypochlorite ion as a major radiolytic byproduct. New experiments will allow us to quantify efficiently the generation rate of this species. The extreme complexity of the studied chemical systems requires us to use the most efficient and recent analytical techniques and methods existing. For this purpose, the Actinide Chemistry team recently undertook the development of a laser spectroscopy device to determine the speciation of actinides in brines at very low concentrations. We are also developing a method for measuring microquantities of hydrogen peroxide in high-strength brine solutions.

External Reviews: None

Collaborators: Mark Walthall, NMSU CEMRC
Deborah Moir, NMSU CEMRC

Publications: None

B. 1 Peer-Reviewed Journal Articles FY 2002

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Appendix B. 5 Citations Indices (Past 15 years)

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Appendix B.6 Professional Society Officer CY2002

AGU Surface Water Committee
B. Newman, Member

Clay Minerals Society
Steve J. Chipera, Chairman, Publications Committee (1998-2002)

Ecological Society of America, Rangeland Ecology Section
David D. Breshears, Chair

International Association of Seismology and Physics of the Earth's Interior
Michael Fehler, Member of Association Commission on Wave Propagation
Thomas Shankland, Member of Association Commission on Physical and Chemical Properties of Materials of the Earth's Interior (1992-Present)

International Association of Volcanology and Chemistry of the Earth's Interior
Grant Heiken, Executive Committee and Past-President (1999-2003)

International Committee on Natural Zeolites
David Bish, President (2002-2006)

International Union of Geodesy and Geophysics
Grant Heiken, Secretary, Geophysical Risk and Sustainability Commission (1999-2003)

Mineralogical Society of America
David Bish, Council (1999-2002)

NATO CCMS National Security Research Team
Gerald L. Geernaert, Member

Society for Exploration Geophysics
Leigh House, Research Committee
Michael Fehler, Research Committee

U. S. National Committee for the Geological Sciences of the National Academies
Grant Heiken, Chair

WHO, WMO / GURME, UN-ECE/TFIAM
Gerald L. Geernaert, Panel Member

Appendix B.7 Editorship of Professional Journals and Memberships on Editorial Advisory Boards CY2002

American Mineralogist
David L. Bish, Special Associate
David T. Vaniman, Book Reviews Editor

Clays and Clay Minerals
David L. Bish, Special Associate Editor

Boundary Layer Meteorology Journal; and Environmental Sciences Library, Kluwer
Gerald L. Geernaert, Associate Editor

Bulletin of the Seismological Society of America
Michael Fehler, Editor-in-Chief
Carol Mark, Managing Editor
Charlotte Rowe, Associate Editor

Geological Society of America Bulletin
W. Scott Baldridge, Associate Editor

Geothermics
Fraser E. Goff, Editorial Advisory Board Member
Gregory A. Valentine, Associate Editor

Journal of Environmental Quality
Michael H. Ebinger, Associate Editor

Journal of Volcanology
Fraser E. Goff, Editorial Advisory Board Member
Gregory A. Valentine, Associate Editor

Pure and Applied Geophysics (PAGEOPH)
Howard J. Patton, Associate Editor

Society of Petroleum Engineers Journal
Dongxiao Zhang, Editorial Board Member

Water Resources Research
Dongxiao Zhang, Associate Editor

Vadose Zone Journal
Brent D. Newman, Associate Editor

Appendix B.8 **Professional Honors, Awards, and Election to National Scientific and Engineering Societies** **CY2002**

Alan Burman Publication Award, Naval Research Laboratory
Gerald L. Geernaert

American Geophysical Union Editors' Citation for Excellence in Scientific Refereeing
Zhimming Lu

Brindley Lecture Award, The Clay Minerals Society
David L. Bish

Planet ReVelle=1998 TA34 (number 13358), International Astronomical Union
Douglas O. ReVelle

Large Team Distinguished Performance Award for Yucca Mountain Project, LANL
David L. Bish
James W. Carey
Steve J. Chipera
Zora V. Dash
Carl S. Davenhall
Paul R. Dixon
Roger C. Eckhardt
Al Aziz Eddebbarh
June Fabryka-Martin
Carl W. Gable
Elizabeth A. Gray
Bradley D. Gundlach
Charles D. Harrington
James L. Hollins
Emil F. Homuth
Dianne K. Hyer
Hemendra N. Kalia
Sharad M. Kelkar
Edward M. Kwicklis
Schon S. Levy
Peter C. Lichtner
Cleoves B. Martinez
Maureen A. McGraw
Arend Meijer
C. Wes Myers
Ronald D. Oliver
Frank V. Perry
Mark T. Peters
Bruce A. Robinson
Wendy E. Soll
Daniel F. Stone
Bryan J. Travis
Greg A. Valentine
Bart J. Vanden Plas

David T. Vaniman
Hari S. Viswanathan
Maryam D. Warnock
Douglas J. Weaver
John A. Wilcox
Giday WoldeGabriel
Andy V. Wolfsberg
James E. Young
George A. Zyvoloski

Scripps Institute of Oceanography; and Copenhagen Global Change University of Copenhagen, Denmark

Gerald L. Geernaert, Adjunct Faculty

Appendix B.9 **Recruitment of New Scientists and Post Doctoral Fellows into EES Division** **CY2002**

Technical Staff Members

James E. Bossert, Ph.D. Atmospheric Science, Colorado State University (1990). Jim returned to EES as the Deputy Group Leader for EES-8 (now EES-2) in May 2002. Prior to this Jim was in D-Division, where he worked as a program coordinator for the National Infrastructure Simulation and Analysis Center (NISAC), which uses agent-based simulation for critical infrastructure protection and homeland security. Prior to September 2001, Jim served on the staff of the Associate Director for Threat Reduction in a joint appointment with the Government Relations Office. As a member of the Threat Reduction Office staff, he became familiar with the entire portfolio of technical programs managed through that office and developed overview, briefing, and budget material on these programs for the Threat Reduction and Government Relations offices. Prior to April 2000, Jim was the Meteorology Team Leader in the Atmospheric and Climate Sciences Group (EES-8), leading and performing technical work in wildfire behavior modeling, regional climate simulation, and understanding flow systems in complex terrain. He came to LANL in 1990.

Jonah J Colman, PhD. Atmospheric Chemistry, University of California at San Diego (1996). Jonah was hired in March 2002 as a Technical Staff Member in EES-2. Before joining EES, Jonah was a Postdoctoral Fellow and Staff Scientist at UC Irvine where he was involved in the NASA missions PEM-Tropics A and B in both an analytical and data analysis capacity. Jonah first came to LANL as a visiting scientist at the IGPP working on chemistry implementation in both ocean and wildfire simulation codes. He was offered a Postdoctoral Fellowship at the Laboratory to implement nonlocal chemistry into the FIRETEC wildfire process model, but declined it after being offered a TSM position. He currently splits his time between working on the FIRETEC model and helping to develop a new code for the modeling of an electromagnetic pulse in the atmosphere.

Beverly A. Crawford, PhD, Chemistry, University of New Mexico (1989). Beverly was hired in August 2002 as a Technical Staff Member in EES-12. Her specialty is molecular and atomic spectroscopy and her background includes more than 12 years experience related to nuclear waste characterization and management. Before joining EES, Beverly worked for the Central Characterization Project (CCP) with Washington group and at Hanford with Fluor as a technical team leader for a group of Organic and Inorganic Analytical Chemists. Beverly was the second general lead site project manager (SPM) for the fledgling CCP group under Washington group management. As CCP SPM, Beverly mentored other SPMs coming into the CCP program and worked to create a foundation of competent SPMs with technical and regulatory expertise to manage regulatory decision-making and data validation in support of characterization activities at 3 DOE sites. While at Hanford, Beverly developed organic chemical analysis capabilities at the site's 222-S Laboratory and taught advanced analytical and physical chemistry topics to graduate students at Washington State University Tri-Cities. Beverly brings broad experience in characterization, chemical spectroscopy, nuclear waste and EPA regulations to the Lab. Her research interests include fiber optic Raman sensor probes, photo-physics and application of new technology to characterization of nuclear waste.

Gerald L. Geernaert (Gary), Ph.D., Atmospheric Sciences, University of Washington, Seattle, Washington (1983). In May 2002 Gary joined the Laboratory as the Center Leader of IGPP Los Alamos. Before coming to Los Alamos, Gary was the Director for the Atmospheric Environment Department of the National Environmental Research Institute in Roskilde, Denmark. He was responsible for program oversight of the Danish air quality monitoring program, the Arctic Monitoring and Assessment Program's atmospheric component, and the weather and air quality forecast system. He has served as a consultant on air quality to China, Malaysia, South Africa, Botswana, Egypt, and Thailand. He has also worked at the Office of Naval Research in Arlington, Virginia, the Center for Advanced Space Sensing, US Naval Research Laboratory in Washington DC, Space Systems Technology Department, Navy Center for Space Technology, Office of Strategic Planning, Space Sensing and Applications Branch. His specializations include: program management, personnel management, R&D management, and laboratory management; research policy, science, technology, innovation policy, and environmental policy; air-sea interaction theory and remote sensing; dynamical meteorology and oceanography, turbulence, and climate change; arctic research on contaminants, source-receptor relationships, and policy analysis; Third world environmental strategies, trends, and environmental policy development; and national security: NATO and US-DoD/DOE. Gary has also been appointed as a program manager for the Office of Basic Energy Research (OBER)—Atmospheric Sciences.

Anne K. Hallman, CHP, ME (Master in Engineering), Environmental Engineering, University of Florida (1988). Anne was hired in August 2002 as a Technical Staff Member in EES-12 Her specialty is health physics and radioactive waste management, and her background includes more than ten years experience in radioactive waste projects. Anne's past experience includes 13 years at Sandia National Laboratories where she filled various positions as a project leader and Principal Member of Technical Staff. Anne is a certified health physicist and she brings broad experience in low-level, mixed low-level, and TRU radioactive waste management, as well as emergency operations support to the Lab.

Jerri Lynne McTaggart, BS, Biology Lamar University (1977). Jerri was hired May 6, 2002 as TSM in EES-12. Her specialty is Waste Characterization and she has spent over eighteen years in the nuclear industry. Jerri came from Rocky Flats where she supervised crews in waste characterization, repackaging foaming operations, Visual Exam, Non-Destructive Exam, Non-Destructive Assay, chemical management, and plutonium packaging and shipping operations. She designed and engineered several repackaging systems to accommodate legacy wastes. Jerri is interested in finishing the Masters she started in Denver for Environmental Policies and Management.

Laurie Sparks-Roybal, PhD, Chemistry, University of New Mexico (1992). Laurie was hired in December 2002 as a Technical Staff Member in EES-12. Her specialty is molecular and atomic spectroscopy, TRU waste characterization, and regulatory compliance regarding the WIPP. Her background includes more than 10 years experience related to nuclear waste characterization and management, and more than 8 years experience with WIPP compliance. Before joining EES, Laurie worked for the Institute for Regulatory Science (RSI), for the Central Characterization Project (CCP) with Washington group, for the TRU waste characterization/certification program (TWCP) at Los Alamos National Laboratory, and at Hanford with Westinghouse Hanford Company (now Fluor). With RSI, Laurie participated in peer review and stakeholder outreach activities, and conducted research regarding TRU waste characterization activities used throughout the DOE TRU waste complex. Laurie served as the National Certification Team Manager and as the first Site Project Manager for the CCP under Washington group management at WIPP. In these positions, she participated in the development and implementation of CCP activities at three DOE sites. At LANL, Laurie was the Deputy Site Project Manager for the

TWCP, when LANL sent the first shipment of TRU waste to open the WIPP in March 1999. While at Hanford, Laurie was responsible for laboratory elemental analysis of hazardous, radioactive waste using atomic absorption methods at the site's 222-S Laboratory. Laurie also developed bench top FTIR and Raman spectrometers for mobile waste characterization and provided comprehensive instrument validations, technical support and field assistance for a portable, open-path, FTIR spectrometer for Hanford site air monitoring projects.

Richard J Stead, PhD, Geophysics, California Institute of Technology (1990). Richard was hired in December 2002 as a Technical Staff Member in EES-11. His specialty is seismology, and his background includes more than 12 years experience related to nuclear explosion monitoring. Before joining EES, Richard worked for SAIC at the Department of Defense's Center for Monitoring Research, where he filled various positions including Director of Operations and Principal Scientist, and played a key role in creating and operating the systems that monitor the Comprehensive Nuclear Test Ban Treaty. He brings broad experience in monitoring operations and systems to the Lab. His research interests include sensor arrays, wave propagation and source characterization.

Julia Whitworth, BA, Chemistry and Mathematics; MS, Hydrogeology, New Mexico Institute of Mining and Technology (1997). Additionally, Julia is a Master Level Certified Hazardous Materials Manager (CHMM). Julia was hired in November 2002 as a Technical Staff Member in EES-12. Julia has approximately 15 years of experience in hazardous and radioactive waste management, regulatory compliance, and environmental restoration. She has managed hazardous and radioactive waste characterization and management operations at numerous different sites including Coors Brewing Company, Kennecott Copper, Brigham Young University, Motorola, Shell Oil, and Sandia National Laboratories. She is currently performing TRU waste characterization work for Los Alamos National Laboratories. Other major projects have included work in Ukraine for the ICBM Dismantlement Program, RCRA Part B permit preparation for the Savannah River Site and Umatilla Army Depot, and groundwater cleanup projects for Ryder Truck and Williams AFB near Phoenix, AZ.

Postdoctoral Fellows/Research Associates

Donatella Pasqualini, Ph.D., Physics, University of Trento, Italy (2001). Donatella joined EES 11 as a Postdoctoral Research Associate, working with Paul Johnson and Steen Rasmussen. Her dissertation was entitled: "Collective Properties of Simple and Molecular Liquids." The thesis dealt with the microscopic dynamics of simple and molecular liquids, studying structural and dynamical properties by computer simulations. In the case of simple liquids, a comparison with experimental measurements (neutron scattering) was performed. The main goal of this work was to understand the effects of the interaction potential and the thermodynamic state on the collective dynamical properties of liquids. The systems analyzed were a simple liquid, Rubidium, an alkali metal liquid, and HCl, as a molecular liquid. Recently, Pasqualini has contributed to modeling efforts for understanding Atomic Fast Nonlinear Dynamics (AFND) via simulation of stochastically driven chains. Pasqualini's general research interests lie in complex phenomena and modeling of complex phenomena by molecular dynamics. In 2002, together with S. Habib and K. Heitmann, she has collaborated on a new theoretical paradigm for understanding AFND and slow dynamics (SD) in geomaterials and begun numerical implementations of stochastic models.

Jean-Francois Lucchini, Ph.D. Chemistry, specialization Radiochemistry, University of Paris XI, France (2001). Jean-Francois joined EES-12 in Carlsbad in September 2002, as a Postdoctoral Research Associate, to work on the Actinide Chemistry and Repository Science Program in support of the Waste Isolation Pilot Plant. The focus of his study is to better understand the complex chemistry of actinides elements, especially uranium and plutonium, in brine solutions in the presence of radiolytic by-products. Jean-Francois is performing two types of experiments: speciation experiments at the Carlsbad Environmental Monitoring & Research Center (CEMRC) of New Mexico State University (NMSU), and radiolysis experiments at the Ion Beam Facility of MST-8 in Los Alamos. He is also developing spectroscopic methodologies for the new EES-12 Nd-Yag laser. During his Ph.D. thesis, Jean-Francois studied Water Alpha-Radiolysis Effects on UO_2 Alteration at two Nuclear Research Centres of the Commissariat a l'Energie Atomique (CEA–France).

Andrew V. Newman, Ph.D. Geological Sciences, specialization in Geophysics, Northwestern University, Evanston, IL (2000). Andrew came to EES-9 in September 2002 as a Director's Postdoctoral Fellow to develop advanced numerical models of deformation in silicic volcanic systems using viscoelastic rheologies. The focus of this study concentrates on Long Valley Caldera in Eastern California because of the abundant existing deformation data there, however, Andrew is performing pilot GPS deformation studies of both the Valles Caldera (immediately west of LANL) and the Socorro Magma Body (beginning 50 km south of Albuquerque), to determine if there exists suitable deformation signals to monitor more closely. For his Ph.D. thesis, Andrew used GPS deformation and existing seismological data to assess realistic earthquake recurrence estimates and alternative probabilistic earthquake hazard maps for the New Madrid seismic zone. For the two years prior to coming to LANL, Andrew, as a postdoctoral Researcher at the University of California Santa Cruz, has been working on a joint seismological and geodetic experiment in Costa Rica to establish a more complete understanding of the coupling between subducting oceanic and overriding continental lithosphere, the region where most of the world's great earthquakes occur.

Andrzej J. Rafalski, Ph.D. Chemistry, specialization in Radiation Chemistry of Polymers, Institute of Nuclear Chemistry and Technology, Warsaw, Poland (1999). Andrzej came to EES-12 in Carlsbad on October 2002 as a Postdoctoral Research Associate to develop a unique method of hydrogen peroxide concentration measurement in the presence of hypochlorite, in sodium and magnesium brines. In a nuclear waste repository such as WIPP, the radiation from the wastes can produce hydrogen peroxide and hypochlorite as by-products in brine solutions, which could influence the actinide speciation and solubility, changing the performance of the repository. The evaluation of hydrogen peroxide concentration is essential for further study and understanding the actinide behavior in irradiated brines. For the three years prior to coming to LANL, Andrzej has been studying the decomposition of virgin polypropylene at moderate temperatures and the radiolysis of polymers by means of DRS (Diffuse Reflection Spectrophotometry) at Institute of Nuclear Chemistry and Technology.

Charlotte A. Rowe, Ph. D., Earth and Environmental Science with dissertation in geophysics, New Mexico Institute of Mining and Technology, Socorro, NM (2000). Charlotte came to EES-11 in August 2002 to work with the Nuclear Explosion Monitoring team as a Postdoctoral Research Associate. The waveform cross-correlation and precise location and source discrimination expertise she gained during her Ph. D. studies have direct applications to problems currently being investigated by the Nuclear Explosion Monitoring team. In addition to signal processing and automatic classification work, Charlotte has spent nineteen years researching and monitoring active volcanoes from Antarctica to Alaska to the Caribbean. She spent two years working with 3D seismic oil exploration in the International Division of Geophysical Service, Inc., and acted as teaching assistant and instructor for geophysical exploration classes and field camps in Alaska and New Mexico. Charlotte also serves as an Associate Editor for the Bulletin of the Seismological Society of America.

Chad C. Schmidt, Ph.D., Mechanical Engineering, Stanford University (2000). His thesis project was the study of the Thermal De-NOx reaction at high pressures.□Chad came to LANL as a Postdoctoral Research Associate in November of 2000 and worked in ESA-WMM.□During his two-year stay in that group, he worked on a boundary element model as part of the ASCI project and lifetime extension program.□He was also involved in projects to measure aerosol optical properties and collect air samples from plumes.□Chad transferred to EES-2 in December 2002 for the third year of his postdoc.□Currently, he is working on the "Water On Mars" project, and is using the HIGRAD model to simulate the seasonal behavior of the Mars polar CO_2 caps.